Feature-Based Aggregation and Deep Reinforcement Learning

Dimitri P. Bertsekas

Laboratory for Information and Decision Systems
Massachusetts Institute of Technology

Arizona State University

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AlphaZero Program (2017)

AlphaZero

Plays much better than all chess programs
Plays different!
Learned from scratch ... with 4 hours of training!
Same algorithm learned multiple games (Go, Shogi)
AlphaZero was Trained Using Self-Generated Data

AlphaZero implements a form of policy iteration/approximate DP method

- Generates a sequence of players/policies, each implemented by a deep neural net
- A player’s games are used to train an “improved” player (self-learning)
- The neural net of a player/policy provides at any position: the "value" of the position, and a “probabilistic ranking" of the possible moves
- The games of a player are generated by Monte-Carlo Tree Search (MCTS, a form of randomized multistep lookahead)
- Training uses a form of regression
- AlphaZero bears similarity to earlier works, e.g., TD-Gammon (Tesauro,1992), but is more complicated because of the MCTS and the deep NN
Exact DP applies (in principle) to a very broad range of optimization problems:

- Deterministic $\leftarrow$ Stochastic
- Combinatorial optimization $\leftarrow$ Optimal control w/ infinite state/control spaces
- One decision maker $\leftarrow$ Two player games
- ... BUT is plagued by the curse of dimensionality and need for a math model

Approximate DP/Reinforcement Learning:

- Overcomes the difficulties of exact DP by using:
  - Approximation (to reduce dimension)
  - Simulation (in place of a math model)
- Can be used in a very broad range of challenging/large scale problems
- Has proved itself in many fields ...
- ... BUT implementation is a challenge/art and success is not guaranteed
- Still there is theory that guides the art
A Summary

Some History

- **1950s-60s**: Bellman (DP), Shannon (chess), Samuel (checkers)
- **80s-early 90s**: Approximation and simulation-based methods: Barto/Sutton [TD(\(\lambda\)), AI-DP connection], Watkins (Q-learning), Tesauro (backgammon, self-learning)
- **1990s**: Rigorous analysis, mathematical understanding, first books
- **Late 90s-Present**: Rollout, Monte-Carlo Tree Search, Deep Neural Nets, Model Predictive Control

Methodology

- **Math framework is DP** (plus function approximation, training by simulation)
- Approximations in value space and in policy space (compact/low-dimensional, feature-based parametric architectures)
- **Supervised vs unsupervised learning** (using external vs self-generated data)
- **No dominant method.** Some ideas are solid and some are heuristic
- **Success depends on finding the right mix of implementation ideas**, and using massive computational power
- The AlphaZero program combines in a skillful way ideas that have been known since around 2005
Purpose of this Talk

Selectively survey the state of the art with focus on:
- Approximate policy iteration
- Neural network implementations
- Aggregation

Describe the relevant contributions of neural networks:
- Provide an approximation architecture for the cost function of a policy
- Automatically construct the features of the architecture using self-generated data
- Use in neural network-based policy iteration

Describe the feature-based aggregation methodology, and how it can be used in combination with neural nets
References

**Survey paper**


**DP/RL Book references**

- Bertsekas and Tsitsiklis, Neuro-Dynamic Programming, 1996
- Sutton and Barto, Reinforcement Learning, 1998 (2nd ed. on-line, 2018)

**My latest theoretical monograph on DP**

Bertsekas, Abstract Dynamic Programming: 2nd edition, 2018
RL uses Max/Value, DP uses Min/Cost

- Reward of a stage = (Opposite of) Cost of a stage.
- State value = (Opposite of) State cost.
- Value (or state-value) function = (Opposite of) Cost function.

Controlled Markov chain terminology

- Agent = Controller or decision maker.
- Action = Control.
- Environment = System.

Methods terminology

- Learning = Solving a DP-related problem using simulation.
- Self-learning (or self-play in the context of games) = Solving a DP problem using simulation-based policy iteration.
- Planning vs Learning distinction = Solving a DP problem with math model-based vs model-free simulation.
- Prediction = Policy evaluation.
1. Exact and Approximate Policy Iteration
2. Approximate Policy Evaluation with Neural Nets
3. Feature-Based Aggregation
4. Feature-Based Aggregation with Neural Networks
Discounted Infinite Horizon Problem

Transition probabilities $p_{ij}(u)$
Cost $\alpha^k g(i, u, j)$

 Controlled Markov Chain

A Markov chain with states 1, \ldots, n, and control $u$

- $p_{ij}(u)$: Transition probability from $i$ to $j$ under $u$
- $\alpha^k g(i, u, j)$: Cost of the $k$th transition; $\alpha \in (0, 1)$: discount factor

Policy (or feedback controller) $\mu$: Maps each state $i$ to a control $\mu(i)$

- Total cost of $\mu$ starting at $i_0$: $J_\mu(i_0) = E \left\{ \sum_{k=0}^{\infty} \alpha^k g(i_k, \mu(i_k), i_{k+1}) \right\}$
- Optimal cost starting at $i_0$: $J^*(i_0) = \min_\mu J_\mu(i_0)$
- Optimal policy $\mu^*$: Satisfies $J_{\mu^*}(i) = J^*(i)$ for all $i$
### Basic Theory

#### Bellman’s equation for $J^*$

$$J^*(i) = \min_u \sum_{i=1}^{n} p_{ij}(u) \{ g(i, u, j) + \alpha J^*(j) \}, \quad \text{for all } i$$

Optimal cost at $i = \min_u E\{1{\text{st stage exp. cost}} + \text{optimal cost of remaining stages}\}$

#### Policy evaluation (Bellman) equation for the cost function $J_\mu$ of a given policy $\mu$

$$J_\mu(i) = \sum_{i=1}^{n} p_{ij}(\mu(i)) \{ g(i, \mu(i), j) + \alpha J_\mu(j) \}, \quad \text{for all } i$$

#### Policy improvement principle

Given a policy $\mu$ and its evaluation $J_\mu$, we can obtain an improved policy $\hat{\mu}$ through

$$\hat{\mu}(i) = \arg \min_u \sum_{i=1}^{n} p_{ij}(u) \{ g(i, u, j) + \alpha J_\mu(j) \}, \quad \text{for all } i$$

We have $J_{\hat{\mu}}(i) \leq J_\mu(i)$ for all $i$
Exact policy iteration is successive policy improvement:

\[ \mu_0 \Rightarrow \mu_1 : \text{improved policy over } \mu_0 \Rightarrow \mu_2 : \text{improved policy over } \mu_1 \Rightarrow \cdots \]

We have \( J_{\mu_k} \rightarrow J^* \).

Approximate policy iteration is policy improvement w/ approximate evaluation:

\[ \mu_0 \Rightarrow \mu_1 : \text{“improved” policy over } \mu_0 \Rightarrow \mu_2 : \text{“improved” policy over } \mu_1 \Rightarrow \cdots \]

“Converges” to optimum within an error bound [of order \( O((1 - \alpha)^2) \) or \( O((1 - \alpha)) \)].
Feature-Based Policy Evaluation

Features $F$ and weights $r$ provide a lower-dimensional representation of $J_{\mu}$

- The features can be viewed as basis functions
- The weights depend on $\mu$ (sometimes the features also)
- Critical question: How to find good features?
  - Handcrafted, based on a priori knowledge/intuition
  - Constructed from data, e.g., using a neural network (this is the BIG contribution of NNs)

Approximation in a space of basis functions

$\tilde{J}_{\mu}(F(i), r)$: Feature-based parametric architecture

$F(i) = (F_1(i), \ldots, F_s(i))$: Vector of Features of $i$

$r$: Vector of weights
NN-Based Evaluation of $\tilde{J}_\mu$ for a Given Policy $\mu$

Generate state-cost samples $(i_m, \beta_m), m = 1, \ldots, M, \beta_m = J_\mu(i_m) + \text{"noise"}$

- Use **nonlinear optimization/regression**: Find $(v, r)$ that minimizes
  \[
  \sum_{m=1}^{M} (\tilde{J}_\mu(i_m, v, r) - \beta_m)^2
  \]

- Use of an **incremental gradient method** (also called SGD, backpropagation)
- Making the method work is an art (regularization, hot start, stepsize, etc)
- **Universal approximation** theorem
- To generate the cost samples: We simulate the Markov chain under $\mu$
- We can use alternative regressions (e.g., based on temporal differences, etc)
A deep NN just has many layers

- Can be viewed as providing a “hierarchy of features"
- The last set of features is the one used in the cost approximation
- More “sophisticated” features with each stage, fewer weights needed (?)
- Sampling and training is the same as in single layer nets
- Is deeper better? Tesauro’s and subsequent backgammon implementations used one nonlinear layer!
- For our purposes, deeper is better. There are fewer final features in deep NNs
Basic Principles of Aggregation

An old idea: Problem approximation (rather than algorithm approximation)

- Group “similar” states together and represent them as a single state
- Approximate the original DP problem with a fewer-state DP problem, called aggregate problem
- Solve the aggregate problem and “extend” its cost function to the original
- The aggregate problem can be solved by exact DP and simulation-based methods

A simple example: Approximate a fine grid with a coarse grid

Another example (hard aggregation): Partition the state space into disjoint subsets, each viewed as a single “aggregate state"
Use a Feature Map $F(i)$ to Form the Aggregate DP Problem

Idea: Group together states with “similar” features (i.e., small variation of $F$)

Aggregate states: Disjoint subsets $S_1, \ldots, S_q$ of state-feature pairs $(i, F(i))$

- System states $j$ relate to the aggregate states according to “membership/interpolation weights” $\phi_{1\ell}, \ldots, \phi_{n\ell}$ (called aggregation probabilities)
- Each aggregate state $S_\ell$ relates to its “footprint”, the set $I_\ell = \{ i \mid (i, F(i)) \in S_\ell \}$, according to “importance weights” $d_{\ell 1}, \ldots, d_{\ell n}$ (called disaggregation probabilities)
- Constraints:
  - If $j \in S_\ell$ then $\phi_{j\ell} = 1$ (membership weight 1 for states in the footprint)
  - If $i \not\in I_\ell$ then $d_{\ell i} = 0$ (importance weight 0 for states outside the footprint)
**Aggregate DP Problem: Approximation through Features**

- **States**: Aggregate states plus two copies of the original system states.
- **Costs and transition probabilities**: As shown.
- **Optimal costs**: \( r^*_\ell \) for aggregate state \( S_\ell \), \( \tilde{J}_0(i) \) for left state \( i \), \( \tilde{J}_1(j) \) for right state \( j \).
- By Bellman’s equation for the aggregate problem we have
  \[
  \tilde{J}_1(j) = \sum_{\ell=1}^{q} \phi_{j\ell} r^*_\ell, \quad j = 1, \ldots, n \quad \text{(piecewise linear)}
  \]

Once we compute \( r^*_\ell \), we can obtain an “improved” policy

\[
\hat{\mu}(i) = \min_{u \in U(i)} \sum_{j=1}^{n} p_{ij}(u) \left( g(i, u, j) + \alpha \sum_{\ell=1}^{q} \phi_{j\ell} r^*_\ell \right), \quad i = 1, \ldots, n
\]
Aggregation-Based Approximate Policy Iteration

Initial Policy

Generate Features $F(i)$ of Current Policy $\mu$

Formulate Aggregate Problem

Generate “Improved” Policy $\hat{\mu}$ by “Solving” the Aggregate Problem

Use a Neural Network or Other Scheme
Possibly Include “Handcrafted” Features

Form the Aggregate States
Choose the Aggregation and Disaggregation Probabilities
Properties of the Aggregate Problem

- Aggregate problem lends itself to simulation if the original problem does
- \( r^*_\ell \) is computable with exact/tabular methods, e.g., TD(\(\lambda\)), LSTD, LSPE, Q-learning

Intuition and analysis/error bounds suggest the following general strategy:

Use features that conform to \( J^* \), i.e.,

\[
J^*(i) \approx J^*(i') \implies F(i) \approx F(i')
\]

Form aggregate states so that \( F \) varies little within their footprint
Using “Scoring” Functions

Suppose we have a function $V$ with “similar form” to $J^*$ (up to a constant shift)

- We can use $V$ as a feature map and group states with similar values of $V$
- Each interval may contain one or multiple states
- Many intervals lead to more accurate but more time-consuming solution

Extend this idea to a vector of scoring functions $V(i) = (V_1(i), \ldots, V_s(i))$
Approximate PI with Aggregation and Neural Nets

“Standard” NN-based PI

NN-based PI with aggregation

- Start with a training set of state-cost pairs generated using the current policy $\mu$
- Evaluate $\mu$ using the NN; obtain a feature map $F$, and a sample of $(i, F(i))$ pairs
- Construct aggregate states and a feature-based aggregate problem (essentially use $F$ as a vector scoring function, possibly with some handcrafted features)
- Use as “improved” policy $\hat{\mu}$ the optimal policy of the aggregate problem
- More work for policy improvement, but may yield better “improved” policy
Concluding Remarks

- NNs resolve a major difficulty of approximate PI: **Automatically extract features** of the cost function of a policy.
- Good features, once extracted can be used for other purposes, including aggregation. Deep NNs provide fewer final features, which favors aggregation.
- Aggregation benefits from the solidity of exact DP algorithms.

Some words of caution on approximate PI

- There are challenging implementation issues:
  - Approximation architecture design using features
  - Sample design/explore well the state space
  - Training algorithms
  - Oscillations
  - Recognizing success or failure!

- The RL game successes are spectacular, but they have benefited from **perfectly known and stable models** and relatively **small number of controls** (per state).
- On the positive side, massive computational power together with distributed computation are a source of hope.
- There is an exciting journey ahead ...
Thank you!