Feature-Based Aggregation and Deep Reinforcement Learning

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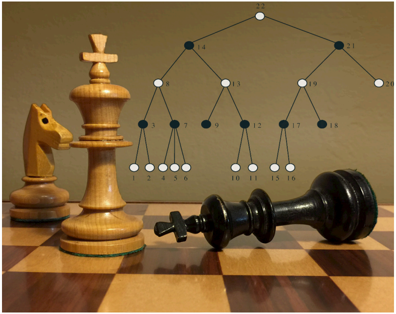


AlphaZero

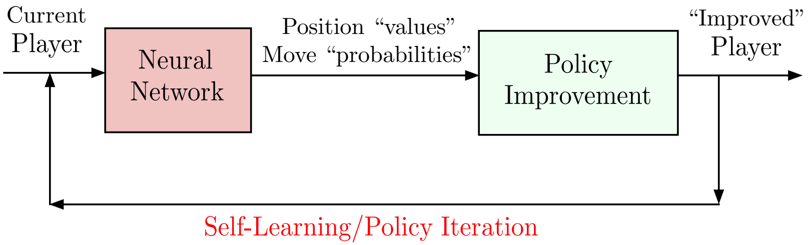
Plays much better than all chess programs

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

DP/RL: A CLASSICAL AND UNIVERSAL METHODOLOGY

Exact DP applies (in principle) to a very broad range of optimization problems

- Deterministic <—-> Stochastic
- Combinatorial optimization <—-> Optimal control w/ infinite state/control spaces
- One decision maker <—-> 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-early90s: Approximation and simulation-based methods: Barto/Sutton [TD(λ), 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

Bertsekas, “Feature-Based Aggregation and Deep Reinforcement Learning: A Survey and Some New Implementations," Lab. for Information and Decision Systems Report, MIT, April 2018; http://arxiv.org/abs/1804.04577

DP/RL Book references

- Bertsekas and Tsitsiklis, Neuro-Dynamic Programming, 1996
- Sutton and Barto, Reinforcement Learning, 1998 (2nd ed. on-line, 2018)
- Bertsekas, Dynamic Programming and Optimal Control: 4th edition, 2017

My latest theoretical monograph on DP

Bertsekas, Abstract Dynamic Programming: 2nd edition, 2018

Relations and Terminology in RL/AI and DP/Control

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

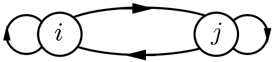
- Learning = Solving a DP-related problem using simulation.
- Self-learning (or self-play in the context of games) = Solving a DP problem using simulation-based policy iteration.
- Planning vs Learning distinction = Solving a DP problem with math model-based vs model-free simulation.
- Prediction = Policy evaluation.

Outline

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 kth transition; $\alpha \in (0, 1)$: discount factor

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

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

Basic Theory

Bellman's equation for J^*

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

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

Policy evaluation (Bellman) equation for the cost function J_μ of a given policy μ

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

Policy improvement principle

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

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

We have $J_{\hat{\mu}}(i) \leq J_\mu(i)$ for all i

Exact and Approximate Policy Iteration (PI)

Exact policy iteration is successive policy improvement:

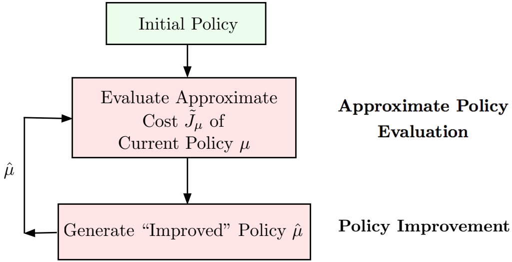
$$\mu_0 \;\Rightarrow\; \mu_1 : \text{improved policy over } \mu_0 \;\Rightarrow\; \mu_2 : \text{improved policy over } \mu_1 \;\Rightarrow\; \cdots$$

We have $J_{\mu_k} \to J^*$.

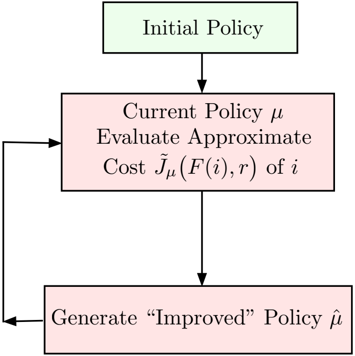
Approximate policy iteration is policy improvement w/ approximate evaluation:

$$\mu_0 \;\Rightarrow\; \mu_1 : \text{“improved" policy over } \mu_0 \;\Rightarrow\; \mu_2 : \text{“improved" policy over } \mu_1 \;\Rightarrow\; \cdots$$

“Converges" to optimum within an error bound [of order $O((1-\alpha)^2)$ or $O((1-\alpha))$].



Feature-Based Policy Evaluation



Approximation in a space of basis functions

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

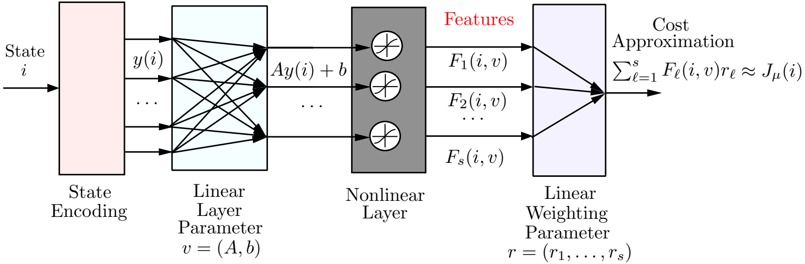
$F(i) = \big(F_1(i), \ldots, F_s(i)\big)$: Vector of Features of i

r: Vector of weights

Features F and weights r provide a lower-dimensional representation of J_μ

- The features can be viewed as basis functions
- The weights depend on μ (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)

NN-Based Evaluation of $\tilde{J}_\mu$ for a Given Policy μ

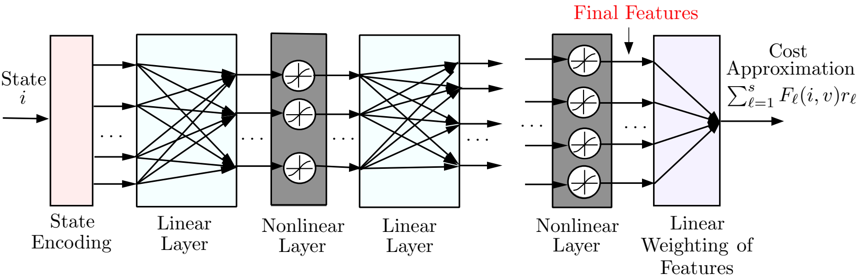


Generate state-cost samples (i_m, β_m), $m=1,\dots,M$, $\beta_m = J_\mu(i_m)$+"noise"

- Use nonlinear optimization/regression: Find (v, r) that minimizes

$$\sum_{m=1}^{M} \big(\tilde{J}_\mu(i_m, v, r) - \beta_m\big)^2$$

- 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 μ
- We can use alternative regressions (e.g., based on temporal differences, etc)



A deep NN just has many layers

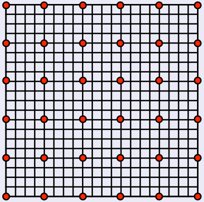
- Can be viewed as providing a “hierarchy of features"
- The last set of features is the one used in the cost approximation
- More “sophisticated" features with each stage, fewer weights needed (?)
- Sampling and training is the same as in single layer nets
- Is deeper better? Tesauro’s and subsequent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

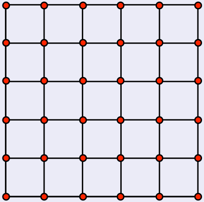
Basic Principles of Aggregation

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

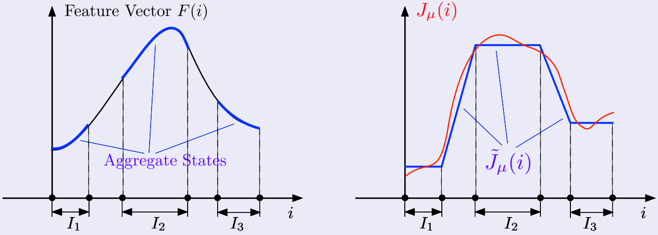




Another example (hard aggregation): Partition the state space into disjoint subsets, each viewed as a single "aggregate state"

Use a Feature Map $F(i)$ to Form the Aggregate DP Problem

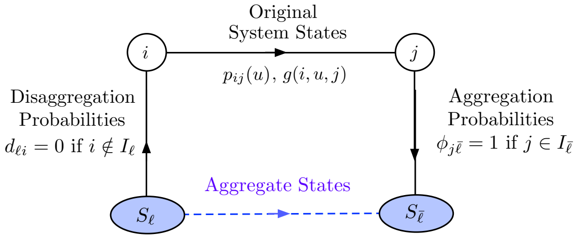
Idea: Group together states with “similar" features (i.e., small variation of F)



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_ℓ 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 $i \notin I_\ell$ then $d_{\ell i} = 0$ (importance weight 0 for states outside the footprint)

Aggregate DP Problem: Approximation through Features



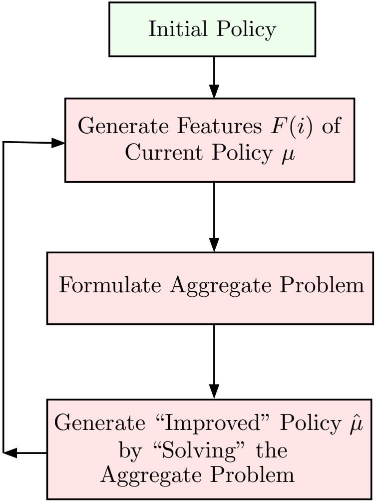
- States: Aggregate states plus two copies of the original system states
- Costs and transition probabilities: As shown
- Optimal costs: r_ℓ^* for aggregate state S_ℓ, $\tilde J_0(i)$ for left state i, $\tilde J_1(j)$ for right state j
- By Bellman's equation for the aggregate problem we have

$$\tilde J_1(j) = \sum_{\ell=1}^{q} \phi_{j\ell} r_\ell^*, \quad j = 1, \ldots, n \qquad \text{(piecewise linear)}$$

- Once we compute r_ℓ^*, we can obtain an "improved" policy

$$\hat\mu(i) = \min_{u \in U(i)} \sum_{j=1}^{n} p_{ij}(u) \left(g(i,u,j) + \alpha \sum_{\ell=1}^{q} \phi_{j\ell} r_\ell^* \right), \qquad i = 1, \ldots, n$$

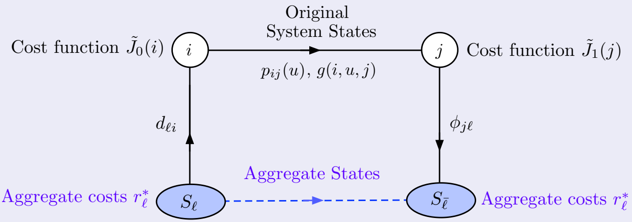
Aggregation-Based Approximate Policy Iteration



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_ℓ^* is computable with exact/tabular methods, e.g., TD(λ), LSTD, LSPE, Q-learning

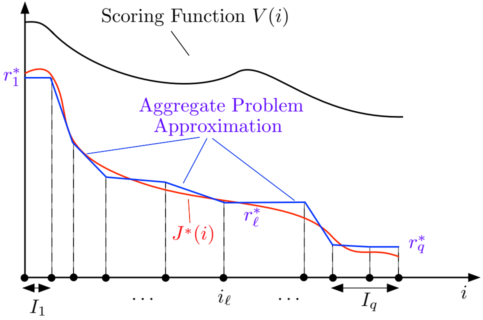
Intuition and analysis/error bounds suggest the following general strategy:

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



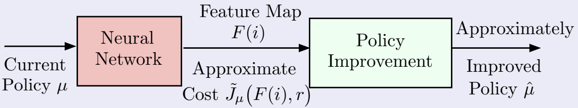
Suppose we have a function V with “similar form" to J^* (up to a constant shift)

- 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

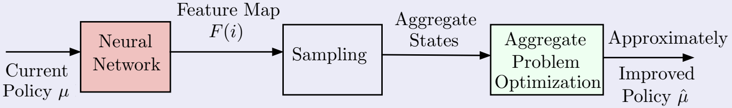
Extend this idea to a vector of scoring functions $V(i) = \big(V_1(i), \dots, V_s(i)\big)$

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 μ
- Evaluate μ using the NN; obtain a feature map F, and a sample of $\big(i, F(i)\big)$ 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!