Topics in Reinforcement Learning: AlphaZero, ChatGPT, Neuro-Dynamic Programming, Model Predictive Control, Discrete Optimization

Arizona State University

Course CSE 691, Spring 2024

Links to Class Notes, Videolectures, and Slides at
http://web.mit.edu/dimitrib/www/RLbook.html

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Lecture 12

More on off-line training, parametric architectures, and their use in approximate value and policy iteration

Aggregation - A different type of parametric architecture

Outline

Approximate Min
Multiagent Min

First Step — "Future"

$$\min_{u_k} E\Big\{ g_k(x_k, u_k, w_k) + \tilde{J}_{k+1}(x_{k+1}) \Big\}$$

Approximate $E\{\cdot\}$
- Certainty equivalence
- Adaptive simulation
- Monte Carlo tree search

Approximate Cost-to-Go $\tilde{J}_{k+1}$
- Problem approximation
- Rollout, Model Predictive Control
- Parametric approximation
- Neural nets
- Aggregation

ONE-STEP LOOKAHEAD

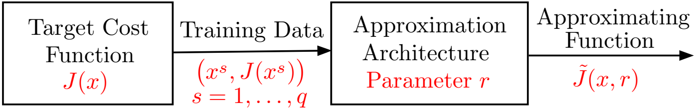
At State x_k
DP minimization

First ℓ Steps — "Future"

$$\min_{u_k, \mu_{k+1}, \ldots, \mu_{k+\ell-1}} E\left\{ g_k(x_k, u_k, w_k) + \sum_{m=k+1}^{k+\ell-1} g_k\big(x_m, \mu_m(x_m), w_m\big) + \tilde{J}_{k+\ell}(x_{k+\ell}) \right\}$$

Lookahead Minimization — **Cost-to-go Approximation**

MULTISTEP LOOKAHEAD



TRAINING CAN BE DONE WITH SPECIALIZED OPTIMIZATION SOFTWARE

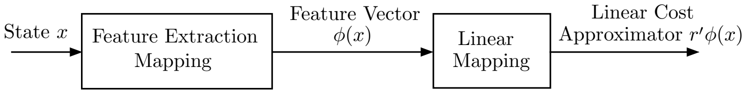
SUCH AS

GRADIENT-LIKE METHODS OR OTHER LEAST SQUARES METHODS

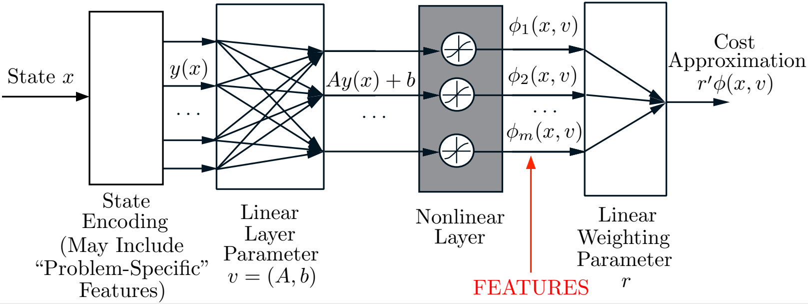
- We select a class of functions $\tilde{J}(x, r)$ that depend on x and a vector $r = (r_1, \ldots, r_m)$ of m "tunable" scalar parameters.
- We adjust r to change $\tilde{J}$ and "match" the training data from the target function.
- Architectures are called linear or nonlinear, if $\tilde{J}(x, r)$ is linear or nonlinear in r.
- Architectures are feature-based if they depend on x via a feature vector $\phi(x)$ that captures "major characteristics" of x,

$$\tilde{J}(x, r) = \hat{J}\big(\phi(x), r\big),$$

  where $\hat{J}$ is some function. Intuitive idea: Features capture dominant nonlinearities.
- A linear feature-based architecture: $\tilde{J}(x, r) = \sum_{\ell=1}^{m} r_\ell \phi_\ell(x) = r'\phi(x)$, where r_ℓ and $\phi_\ell(x)$ are the ℓth components of r and $\phi(x)$.



Neural Nets: An Architecture that Automatically Constructs Features



Given a set of state-cost training pairs (x^s, β^s), $s = 1, \ldots, q$, the parameters of the neural network (A, b, r) are obtained by solving the training problem

$$\min_{A,b,r} \sum_{s=1}^{q} \left(\sum_{\ell=1}^{m} r_\ell \sigma \left(\left(Ay(x^s) + b \right)_\ell \right) - \beta^s \right)^2$$

- Incremental (backpropagation) methods play a critical role.
- Universal approximation; with large enough size, we can approximate "anything."
- Deep neural network advantage; overparametrization helps.

Finite Horizon Sequential DP Approximation - Parametric Approximation at Every Stage (Also Called Fitted Value Iteration)

Train cost approximations $\tilde{J}_N, \tilde{J}_{N-1} \ldots, \tilde{J}_0$, sequentially going backwards

- Start with $\tilde{J}_N = g_N$
- Given a cost-to-go approximation $\tilde{J}_{k+1}$, we use one-step lookahead to construct a large number of state-cost pairs (x_k^s, β_k^s), $s = 1, \ldots, q$, where

$$\beta_k^s = \min_{u \in U_k(x_k^s)} E\Big\{ g(x_k^s, u, w_k) + \tilde{J}_{k+1}\big(f_k(x_k^s, u, w_k), r_{k+1}\big) \Big\}, \qquad s = 1, \ldots, q$$

- We "train" an architecture $\tilde{J}_k$ on the training set (x_k^s, β_k^s), $s = 1, \ldots, q$.
- Each sample involves minimization of an expected value $E\{\cdot\}$

Typical approach: We minimize over r_k

$$\sum_{s=1}^{q} \big(\tilde{J}_k(x_k^s, r_k) - \beta^s\big)^2 \ \ (+ \text{ regularization})$$

Important advantage: Can be combined with on-line play/approximation in value space, so the Newton step interpretation applies. However, $\min_u E\{\cdot\}$ operation complicates the collection of samples.

Fitted Value Iteration with Q-Factors - Model-Free Possibilities

- Consider sequential DP approximation of Q-factor parametric approximations

$$\tilde{Q}_k(x_k, u_k, r_k) \approx E\Big\{g_k(x_k, u_k, w_k) + \min_{u \in U_{k+1}(x_{k+1})} \tilde{Q}_{k+1}(x_{k+1}, u, r_{k+1})\Big\}$$

- We obtain $\tilde{Q}_k(x_k, u_k, r_k)$ by training with many pairs $\big((x_k^s, u_k^s), \beta_k^s\big)$, where β_k^s is a sample of the approximate Q-factor of (x_k^s, u_k^s).
- A mathematical trick: The order of $E\{\cdot\}$ and min have been reversed. Each β_k^s can use a few-samples approximation of the expected value $E\{\cdot\}$.
- Samples β_k^s can be obtained in model-free fashion. Sufficient to have a simulator that generates state-control-cost-next state random samples

$$\big((x_k, u_k), (g_k(x_k, u_k, w_k), x_{k+1})\big)$$

- Having computed r_k, the one-step lookahead control can be obtained on-line as

$$\tilde{\mu}_k(x_k) \in \arg \min_{u \in U_k(x_k)} \tilde{Q}_k(x_k, u, r_k)$$

  without the need of a model or expected value calculations.
- Important advantage: The on-line calculation of the control is simplified.
- However, the Newton step property is lost. Also on-line replanning is lost.
- To address these issues: Use approximation in value space with

$$\tilde{J}_{k+1}(x_{k+1}) = (\text{ or } \approx) \min_u \tilde{Q}_{k+1}(x_{k+1}, u, r_{k+1})$$

Should we Approximate Q-Factors or Q-Factor Differences?

To compare controls at x, we only need Q-factor differences $\tilde{Q}(x,u) - \tilde{Q}(x,u')$

An example of what can happen if we approximate Q-factors:

- Scalar system and cost per stage:

$$x_{k+1} = x_k + \delta u_k, \qquad g(x,u) = \delta(x^2 + u^2), \qquad \delta > 0 \text{ is very small;}$$

  think of discretization of continuous-time problem involving $dx(t)/dt = u(t)$

- Consider policy $\mu(x) = -2x$. Its cost function can be calculated to be

$$J_\mu(x) = \frac{5x^2}{4}(1+\delta) + O(\delta^2), \qquad \text{HUGE relative to } g(x,u)$$

  Its Q-factor can be calculated to be

$$Q_\mu(x,u) = \frac{5x^2}{4} + \delta\left(\frac{9x^2}{4} + u^2 + \frac{5}{2}xu\right) + O(\delta^2)$$

- The important part for policy improvement is $\delta\left(u^2 + \frac{5}{2}xu\right)$. When $Q_\mu(x,u)$ is approximated by $\tilde{Q}_\mu(x,u;r)$, it will be dominated by $5x^2/4$ and will be "lost"
- If we approximate Q-factor differences this problem does not arise

A More General Issue: Disproportionate Terms in Q-Factor Calculations

Remedy: Subtract state-dependent constants from Q-factors (“baselines")

The constants subtracted should affect the offending terms

Example: Consider (truncated) rollout with policy μ and terminal cost function approximation, so $\tilde{J} \approx J_\mu$

- At x, we minimize over u

$$E\{g(x,u,w) + \tilde{J}(f(x,u,w))\}$$

- Question: How to deal with $g(x,u,w)$ being tiny relative to $\tilde{J}\big(f(x,u,w)\big)$? This happens when we time-discretize continuous-time systems. Another case is when costs are “sparse" (e.g., all cost is incurred upon termination).
- A remedy: Subtract $\tilde{J}(x)$ from $\tilde{J}\big(f(x,u,w)\big)$.

Other possibilities (see Sections 3.3.4, 3.3.5 of class notes)

- Learn directly the cost function differences $D_\mu(x,x') = J_\mu(x) - J_\mu(x')$ with an approximation architecture. This is known as differential training.
- Methods known as advantage updating. [Work with relative Q-factors, i.e., subtract the state-dependent baseline $\min_{u'} Q(x,u')$ from $Q(x,u)$.]

Approximate Policy Iteration - α-Discounted Finite-State Problems

Exact PI in finite-state transition probability notation

- Policy evaluation: We compute the cost function J_μ of current policy μ and its Q-factors,

$$Q_\mu(i,u) = \sum_{j=1}^{n} p_{ij}(u)\big(g(i,u,j) + \alpha J_\mu(j)\big), \qquad i = 1,\dots,n,\ u \in U(i)$$

- Policy improvement: We compute the new policy $\overline{\mu}$ according to

$$\overline{\mu}(i) = \arg\min_{u \in U(i)} Q_\mu(i,u), \qquad i = 1,\dots,n.$$

Approximate PI

- Approximate policy evaluation: Introduce a parametric architecture $\tilde{Q}_\mu(i,u,r)$. We determine r by generating a large number of training triplets (i^s, u^s, β^s), $s = 1,\dots,q$, and using a least squares fit:

$$\overline{r} = \arg\min_r \sum_{s=1}^{q} \big(\tilde{Q}_\mu(i^s,u^s,r) - \beta^s\big)^2$$

- Policy improvement: We compute the new policy $\tilde{\mu}$ according to

$$\tilde{\mu}(i) = \arg\min_{u \in U(i)} \tilde{Q}_\mu(i,u,\overline{r}), \qquad i = 1,\dots,n$$

Implementation Issues in Approximate Policy Iteration

BIG challenges to overcome - Rollout is a piece of cake by comparison

Architectural issues:

- To use a linear feature-based architecture, we need to have good features
- To use a neural network, we need to face harder training issues
- For problems with changing system parameters, we need on-line replanning, which may affect the architecture and/or waste the off-line training effort

Inadequate exploration issues:

- To evaluate a policy μ, we must simulate it, so samples of $J_\mu(x)$ are obtained starting from states x frequently visited by μ.
- This underrepresents states x that are unlikely to occur under μ, and throws off the policy improvement.
- Imperfect remedies to this include the use of many short trajectories for generating samples, and occasionally sample with an "off-policy" (a policy other than μ)

Oscillation issues: Policies tend to repeat in cycles

Fascinating phenomena may arise, like "chattering" (convergence in the space of parameters, but oscillation in the space of policies) - they do not arise in aggregation.

Aggregation within the Approximation in Value Space Framework

Approximate minimization

First Step "Future"

$$\min_{u \in U(i)} \sum_{j=1}^{n} p_{ij}(u)\big(g(i,u,j) + \alpha \tilde{J}(j)\big)$$

Approximations:

Replace $E\{\cdot\}$ with nominal values
(certainty equivalence)

Adaptive simulation

Monte Carlo tree search

Computation of $\tilde{J}$:

Problem approximation

Rollout

Approximate PI

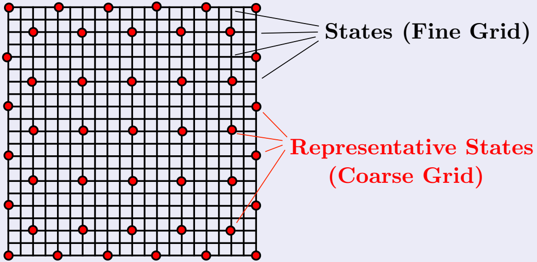
Parametric approximation

Aggregation

- Aggregation is a form of problem approximation. We approximate our DP problem with a "smaller/easier" version, which we solve optimally to obtain $\tilde{J}$.
- Is related to feature-based parametric approximation (e.g., when $\tilde{J}$ is piecewise constant, the features are 0-1 set membership functions).
- Several versions: finite horizon, multistep lookahead, multiagent, etc ...
- Can be combined with parametric approximation (like a neural net) in two ways. Either use the neural net to provide features, or add a local parametric correction to a $\tilde{J}$ obtained by a neural net (see the class notes).

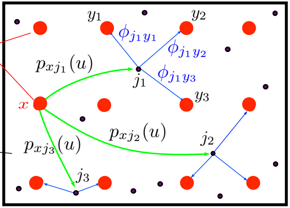
Illustration: A Simple Classical Example of Approximation

Approximate the state space with a coarse grid of states



- Introduce a “small" set of “representative" states to form a coarse grid.
- Approximate the original DP problem with a coarse-grid DP problem, called aggregate problem (need transition probs. and cost from rep. states to rep. states).
- Solve the aggregate problem by exact DP.
- “Extend" the optimal cost function of the aggregate problem to the original fine-grid DP problem, i.e., use some form of interpolation.
- For example extend the solution by a nearest neighbor/piecewise constant scheme (a fine grid state takes the cost value of the “nearest" coarse grid state).

Constructing the Aggregate Problem



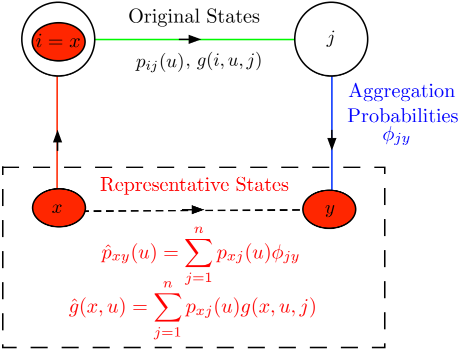
- Introduce a finite subset of "representative states" $\mathcal{A} \subset \{1, \ldots, n\}$. We denote them by x and y.
- Original system states j are related to rep. states $y \in \mathcal{A}$ with aggregation probabilities ϕ_{jy} ("weights" satisfying $\phi_{jy} \geq 0$, $\sum_{y \in \mathcal{A}} \phi_{jy} = 1$).
- Aggregation probabilities express "similarity" or "proximity" of original to rep. states. Can be viewed as interpolation coefficients.
- Aggregate problem dynamics: Transition probabilities between rep. states x, y

$$\hat{p}_{xy}(u) = \sum_{j=1}^{n} p_{xj}(u)\phi_{jy}$$

- Aggregate problem stage cost at rep. state x under control u:

$$\hat{g}(x,u) = \sum_{j=1}^{n} p_{xj}(u) g(x,u,j)$$

The Aggregate Problem - A Reduced State Space DP Problem



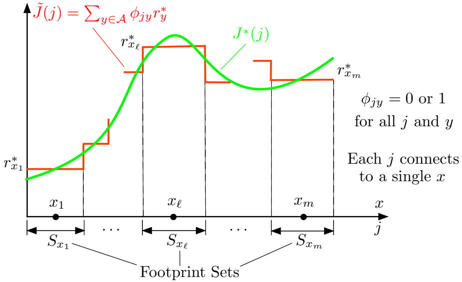
- If r_x^*, $x \in \mathcal{A}$, are the optimal costs of the aggregate problem, approximate the optimal cost function of the original problem by

$$\tilde{J}(j) = \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*, \quad j = 1, \ldots, n, \qquad \text{(interpolation)}$$

- Hard aggregation case: $\phi_{jy} = 0$ or 1 for all j and y. Then $\tilde{J}(j)$ is piecewise constant: It is constant on each set

$$S_y = \{j \mid \phi_{jy} = 1\}, \quad y \in \mathcal{A}, \qquad \text{(called the footprint of } y\text{)}$$

The Hard Aggregation Case ($\phi_{jy} = 0$ or 1 for all j, y)



The approximate cost fn $\tilde{J} = \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*$ is constant at r_y^* within $S_y = \{j \mid \phi_{jy} = 1\}$.

Approximation error for the piecewise constant case ($\phi_{jy} = 0$ or 1 for all j, y)

Consider the footprint sets

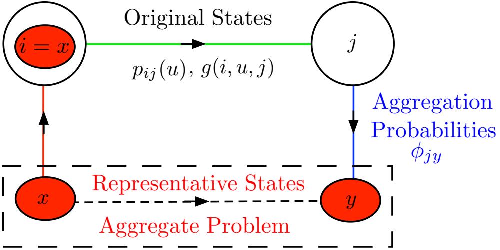
$$S_y = \{j \mid \phi_{jy} = 1\}, \qquad y \in \mathcal{A}$$

Then the $(J^* - \tilde{J})$ error is small if J^* varies little within each S_y. In particular,

$$\big|J^*(j) - \tilde{J}(j)\big| \leq \frac{\epsilon}{1-\alpha}, \qquad j \in S_y,\ y \in \mathcal{A},$$

where $\epsilon = \max_{y \in \mathcal{A}} \max_{i,j \in S_y} \big|J^*(i) - J^*(j)\big|$ is the max variation of J^* within the S_y.

Solution of the Aggregate Problem



Data of aggregate problem (it is stochastic even if the original is deterministic)

$$\hat{p}_{xy}(u) = \sum_{j=1}^{n} p_{xj}(u)\phi_{jy}, \quad \hat{g}(x,u) = \sum_{j=1}^{n} p_{xj}(u)g(x,u,j), \quad \tilde{J}(j) = \sum_{y\in\mathcal{A}} \phi_{jy} r_y^*$$

Exact methods

Once the aggregate model is computed (i.e., its transition probs. and cost per stage), any exact DP method can be used: VI, PI, optimistic PI, or linear programming.

Model-free simulation methods

Given a simulator for the original problem, we can obtain a simulator for the aggregate problem. Then use an (exact) model-free method to solve the aggregate problem.

Extension: Continuous State Space - POMDP Discretization

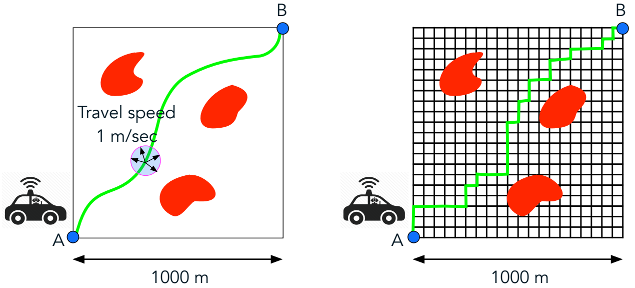
Continuous state space - discounted/bounded cost per stage model

- The rep. states approach applies with no modification.
- The number of rep. states should be finite.
- A simulation/model-free approach may still be used for the aggregate problem.
- We thus obtain a general discretization method for continuous-spaces discounted problems.
- Extension to continuous-state stochastic shortest path problems is more delicate mathematically.

Discounted POMDP with a belief state formulation

- Discounted POMDP models with belief states, fit neatly into the continuous state discounted aggregation framework.
- The aggregate/rep. states POMDP problem is a finite-state MDP that can be solved for r^* with any (exact) model-based or model-free method (VI, PI, etc).
- The optimal aggregate cost r^* yields an approximate cost function $\tilde{J}(j) = \sum_{y \in \mathcal{A}} \phi_{jy} r_y^*$
- $\tilde{J}$ defines a one-step or multistep lookahead suboptimal control scheme for the original POMDP.

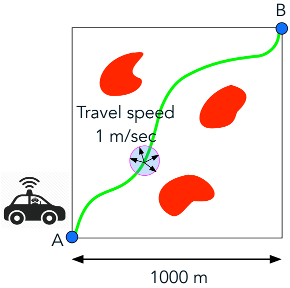
Continuous Control Space Discretization

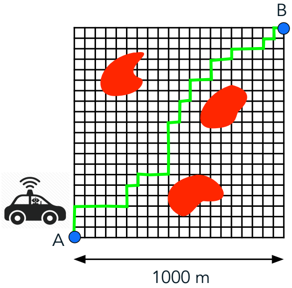


An example: Discretizing Continuous Motion

- A self-driving car wants to drive from A to B through obstacles. Find the fastest route.
- Car speed is 1 m/sec in any direction.
- We discretize the space with a fine square grid. Suppose we restrict the directions of motion to horizontal and vertical.
- We solve the discretized shortest path problem as an approximation to the continuous shortest path problem.
- A challenge question: Is this a good approximation?

Answer to the Challenge Question





Discretizing Continuous Motion

- The discretization is FLAWED.
- Example: Assume all motion costs 1 per meter, and no obstacles.
- The continuous optimal solution (the straight A-to-B line) has length $\sqrt{2}$ kilometers.
- The discrete optimal solution has length 2 kilometers regardless of how fine the discretization is.
- The difficulty here is that the state space is discretized finely but the control space is not.
- This is not an issue in POMDP (the control space is finite).

Aggregation with Representative Features

The main difficulty with rep. states/discretization schemes:

- It may not be easy to find a set of rep. states and corresponding piecewise constant or linear functions that approximate well J^*.
- Too many rep. states may be required for good approximate costs $\tilde{J}(j)$.

Suppose we have a good feature vector $F(i)$: We discretize the feature space

- We introduce representative features that span adequately the feature space
- We aim for an aggregate problem whose states are the rep. features.
- This is a more complicated but also more flexible construction (see the class notes, Section 3.5).