Topics in Reinforcement Learning: Rollout and Approximate Policy Iteration

ASU, CSE 691, Spring 2021

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

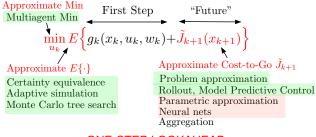
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Lecture 8
Off-Line Training, Neural Nets, and Other Parametric Architectures

Outline

- Parametric Approximation Architectures
- 2 Training of Architectures Switch to Video-Lecture 6 from 2019
- 3 Incremental Optimization of Sums of Differentiable Functions
- Meural Networks
- Neural Nets and Finite Horizon DP
- Back from Video-Lecture 6 from 2019 Miscellaneous Issues in Training

Recall Approximation in Value Space (Mostly Used for On-Line Control Selection)



ONE-STEP LOOKAHEAD



Lookahead Minimization

Approximation

MULTISTEP LOOKAHEAD

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Types of Approximations Used in Off-Line Training

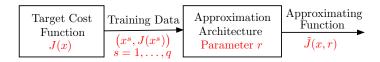
There are two types of off-line approximations in RL:

- Cost approximation in finite and infinite horizon problems
 - Poptimal cost function $J_k^*(x_k)$ or $J^*(x)$, optimal Q-function $Q_k^*(x_k, u_k)$ or $Q^*(x, u)$
 - Cost function of a policy $J_{\pi,k}(x_k)$ or $J_{\mu}(x)$, Q-function of a policy $Q_{\pi,k}(x_k,u_k)$ or $Q_{\mu}(x,u)$
- Policy approximation in finite and infinite horizon problems
 - ▶ Optimal policy $\mu_k^*(x_k)$ or $\mu^*(x)$
 - A given policy $\mu_k(x_k)$ or $\mu(x)$

We will focus on parametric approximations $\tilde{J}(x,r)$ and $\tilde{\mu}(x,r)$

- These are functions of x that depend on a parameter vector r
- An example is neural networks (*r* is the set of weights)

General Parametric Cost Approximation



TRAINING CAN BE DONE WITH SPECIALIZED OPTIMIZATION SOFTWARE SUCH AS

GRADIENT-LIKE METHODS OR OTHER LEAST SQUARES METHODS

Parametric Policy Approximation - Finite Control Space

- If the control has continuous/real-valued components, the training is similar to the cost function case
- If the control comes from a finite control space $\{u^1, \dots, u^m\}$, a modified approach is needed
- View a policy μ as a classifier: A function that maps x into a "category" $\mu(x)$



TRAINING CAN BE DONE WITH CLASSIFICATION SOFTWARE IF THE NUMBER OF CONTROLS IS FINITE

Randomized policies have continuous components
This helps algorithmically

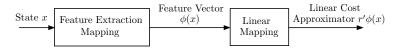
Cost Function Parametric Approximation Generalities

- 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.
- Training the architecture: The algorithm to choose *r* (typically regression-type).
- Local vs global: Change in a single parameter affects \tilde{J} locally vs globally.
- 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,

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

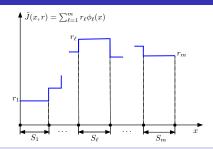
where \hat{J} is some function. Intuitive idea: Features capture dominant nonlinearities.

• 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 ℓ th components of r and $\phi(x)$.



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A Simple Example of a Linear Feature-Based (Local) Architecture



Piecewise constant approximation

• Partition the state space into subsets S_1, \ldots, S_m . Let the ℓ th feature be defined by membership in the set S_ℓ , i.e., the indicator function of S_ℓ ,

$$\phi_{\ell}(x) = \begin{cases} 1 & \text{if } x \in S_{\ell} \\ 0 & \text{if } x \notin S_{\ell} \end{cases}$$

The architecture

$$\widetilde{J}(x,r) = \sum_{\ell=1}^m r_\ell \phi_\ell(x),$$

is piecewise constant with value r_{ℓ} for all x within the set S_{ℓ} .

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Generic Polynomial (Global) Architectures

Quadratic polynomial approximation

- Let $x = (x^1, ..., x^n)$
- Consider features

$$\phi_0(x) = 1, \qquad \phi_i(x) = x^i, \qquad \phi_{ij}(x) = x^i x^j, \quad i, j = 1, \dots, n,$$

and the linear feature-based approximation architecture

$$\tilde{J}(x,r) = r_0 + \sum_{i=1}^n r_i x^i + \sum_{i=1}^n \sum_{j=i}^n r_{ij} x^j x^j$$

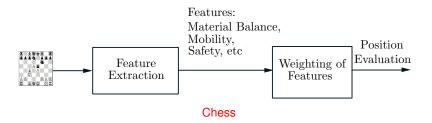
• Here the parameter vector r has components r_0 , r_i , and r_{ii} .

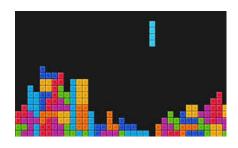
General polynomial architectures: Polynomials in the components x^1, \ldots, x^n

An even more general architecture: Polynomials of features of *x*

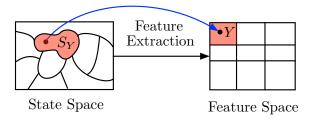
A linear feature-based architecture is a special case

Examples of Problem-Specific Feature-Based Architectures





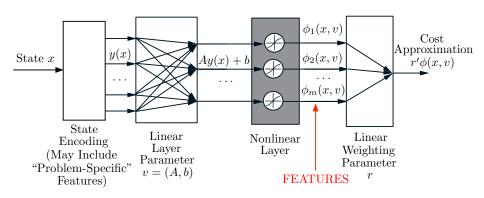
Architectures with Partitioned State Space



A simple method to construct complex approximation architectures:

- Partition the state space into several subsets and construct a separate cost approximation in each subset.
- Can use a separate architecture on each set of the partition.
- It is often a good idea to use features to generate the partition. Rationale:
 - We want to group together states with similar costs
 - We hypothesize that states with similar features should have similar costs

Neural Networks: An Architecture that Works with No Knowledge of Features



A SINGLE LAYER NEURAL NETWORK

Training of Architectures

Least squares regression

- Collect a set of state-cost training pairs (x^s, β^s) , s = 1, ..., q, where β^s is equal to the target cost $J(x^s)$ plus some "noise".
- r is determined by solving the problem

$$\min_{r} \sum_{s=1}^{q} \left(\tilde{J}(x^{s}, r) - \beta^{s} \right)^{2}$$

• Sometimes a quadratic regularization term $\gamma ||r||^2$ is added to the least squares objective, to facilitate the minimization (among other reasons).

Training of linear feature-based architectures can be done exactly

- If $\tilde{J}(x,r) = r'\phi(x)$, where $\phi(x)$ is the *m*-dimensional feature vector, the training problem is quadratic and can be solved in closed form.
- The exact solution of the training problem is given by

$$\hat{r} = \left(\sum_{s=1}^{q} \phi(x^s)\phi(x^s)'\right)^{-1} \sum_{s=1}^{q} \phi(x^s)\beta^s$$

• This requires a lot of computation for a large *m* and data set; may not be best.

Training of Nonlinear Architectures

The main training issue

How to exploit the structure of the training problem

$$\min_{r} \sum_{s=1}^{q} \left(\tilde{J}(x^{s}, r) - \beta^{s} \right)^{2}$$

to solve it efficiently.

Key characteristics of the training problem

- Possibly nonconvex with many local minima, horribly complicated graph of the cost function (true when a neural net is used).
- Many terms in the least least squares sum; standard gradient and Newton-like methods are essentially inapplicable.
- Incremental iterative methods that operate on a single term $(\tilde{J}(x^s, r) \beta^s)^2$ at each iteration have worked well enough (for many problems).

Incremental Gradient Methods

Generic sum of terms optimization problem

Minimize

$$f(y) = \sum_{i=1}^{m} f_i(y)$$

where each f_i is a differentiable scalar function of the n-dimensional vector y (this is the parameter vector in the context of parametric training).

The ordinary gradient method generates y^{k+1} from y^k according to

$$y^{k+1} = y^k - \gamma^k \nabla f(y^k) = y^k - \gamma^k \sum_{i=1}^m \nabla f_i(y^k)$$

where $\gamma^k > 0$ is a stepsize parameter.

The incremental gradient counterpart

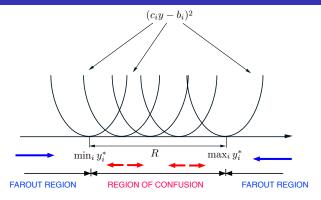
Choose an index ik and iterate according to

$$y^{k+1} = y^k - \gamma^k \nabla f_{i_k}(y^k)$$

where $\gamma^k > 0$ is a stepsize parameter.

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The Advantage of Incrementalism: An Interpretation from the NDP Book



Minimize
$$f(y) = \frac{1}{2} \sum_{i=1}^{m} (c_i y - b_i)^2$$

Compare the ordinary and the incremental gradient methods in two cases

- When far from convergence: Incremental gradient is as fast as ordinary gradient with 1/m amount of work.
- When close to convergence: Incremental gradient gets confused and requires a diminishing stepsize for convergence.

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Incremental Aggregated and Stochastic Gradient Methods

Incremental aggregated method aims at acceleration

- Evaluates gradient of a single term at each iteration.
- Uses previously calculated gradients as if they were up to date

$$y^{k+1} = y^k - \gamma^k \sum_{\ell=0}^{m-1} \nabla f_{i_{k-\ell}}(y^{k-\ell})$$

Has theoretical and empirical support, and it is often preferable.

Stochastic gradient method (also called stochastic gradient descent or SGD)

- Applies to minimization of $f(y) = E\{F(y, w)\}$ where w is a random variable
- Has the form

$$y^{k+1} = y^k - \gamma^k \nabla_y F(y^k, w^k)$$

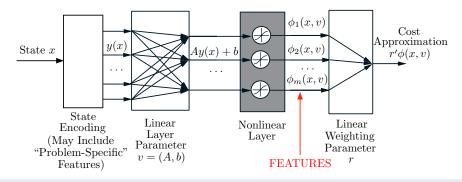
where w^k is a sample of w and $\nabla_y F$ denotes gradient of F with respect to y.

• The incremental gradient method with random index selection is the same as SGD [convert the sum $\sum_{i=1}^{m} f_i(y)$ to an expected value, where i is random with uniform distribution].

Implementation Issues of Incremental Methods - Alternative Methods

- How to pick the stepsize γ^k (usually $\gamma^k = \frac{\gamma}{k+1}$ or similar).
- How to deal (if at all) with region of confusion issues (detect being in the region of confusion and reduce the stepsize).
- How to select the order of terms to iterate (cyclic, random, other).
- Diagonal scaling (a different stepsize for each component of y).
- Alternative methods (more ambitious): Incremental Newton method, extended Kalman filter (see the textbook and references).

Neural Nets: An Architecture that Automatically Constructs Features



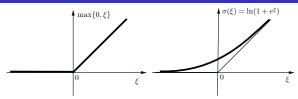
Given a set of state-cost training pairs (x^s, β^s) , s = 1, ..., q, the parameters of the neural network (A, b, r) are obtained by solving the training problem

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

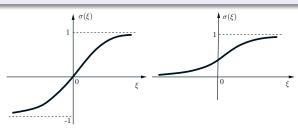
- Incremental gradient is typically used for training.
- Universal approximation property.

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Rectifier and Sigmoidal Nonlinearities



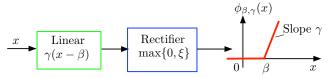
The rectified linear unit $\sigma(\xi) = \ln(1 + e^{\xi})$. It is the rectifier function $\max\{0,\xi\}$ with its corner "smoothed out."



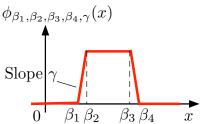
Sigmoidal units: The hyperbolic tangent function $\sigma(\xi) = \tanh(\xi) = \frac{e^{\xi} - e^{-\xi}}{e^{\xi} + e^{-\xi}}$ is on the left. The logistic function $\sigma(\xi) = \frac{1}{1+e^{-\xi}}$ is on the right.

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A Working Break: Challenge Question

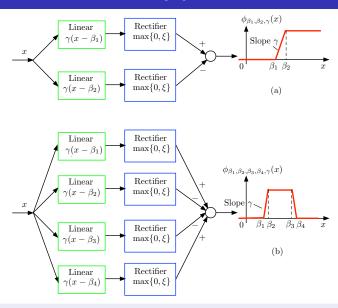


How can we use linear and rectifier units to construct the "pulse" feature below?



- What are the features that can be produced by neural nets?
- Why do neural nets have a "universal approximation" property?

Answer



Using the pulse feature as a building block, any feature can be approximated

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

Start with $\tilde{J}_N = g_N$ and sequentially train going backwards, until k = 0

• 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) , $s = 1, \dots, q$, where

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

• We "train" an architecture \tilde{J}_k on the training set (x_k^s, β_k^s) , $s = 1, \dots, q$.

Typical approach: Train by least squares/regression and possibly using a neural net

We minimize over r_{k}

$$\sum_{k=1}^{q} \left(\tilde{J}_k(x_k^s, r_k) - \beta^s \right)^2$$

Sequential Q-Factor Approximation

Consider sequential DP approximation of Q-factor parametric approximations

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

(Note a mathematical magic: The order of $E\{\cdot\}$ and min have been reversed.)

- We obtain $\tilde{Q}_k(x_k, u_k, r_k)$ by training with many pairs $((x_k^s, u_k^s), \beta_k^s)$, where β_k^s is a sample of the approximate Q-factor of (x_k^s, u_k^s) . [No need to compute $E\{\cdot\}$.]
- Note: No need for a model to obtain β_k^s . Sufficient to have a simulator that generates state-control-cost-next state random samples

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

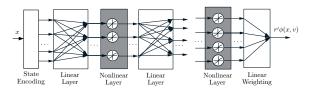
• Having computed r_k , the one-step lookahead control is obtained on-line as

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

without the need of a model or expected value calculations.

Important advantage: The on-line calculation of the control is simplified.

On The Mystery of Deep Neural Networks



- Extensive research has gone into explaining why they are more effective than shallow neural nets for some problems.
- Recent research strongly suggests that overparametrization (many more parameters than data) is the main reason.
- Generally the ratio

$$R = \frac{\text{Number of weights}}{\text{Number of data points}}$$

affects the quality of the trained architecture.

- If $R \approx 1$, the architecture tends to fit very well the training data (overfitting), but do poorly at states outside the data set. This is well-known in machine learning.
- For *R* considerably larger than 1 this problem can be overcome.
- See the research literature and the recent text by Hardt and Recht, 2021, "Patterns, Predictions, and Actions", arXiv preprint arXiv:2102.05242

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 do not use Q-factor differences:

Scalar system and cost per stage:

$$x_{k+1} = x_k + \delta u_k$$
, $g(x, u) = \delta(x^2 + u^2)$, $\delta > 0$ 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

$$J_{\mu}(x) = \frac{5x^2}{4}(1+\delta) + O(\delta^2),$$
 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 $\delta(u^2 + \frac{5}{2}xu)$. 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"

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 (such as \tilde{J})

Example: Consider rollout with cost function approximation $\widetilde{J}pprox J_{\mu}$

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 $\tilde{J}(f(x, u, w))$? An important case where this happens: Time discretization of continuous-time systems.
- A remedy: Subtract $\tilde{J}(x)$ from $\tilde{J}(f(x, u, w))$ (see Section 2.3 of the class notes).

Other possibilities:

- 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).]

About the Next Lecture

We will cover:

- Infinite horizon theory and algorithms
- Discounted and stochastic shortest path problems

PLEASE REVIEW THE INFINITE HORIZON MATERIAL OF THE CLASS NOTES
WATCH VIDEO LECTURE 7 OF 2019 COURSE OFFERING AT MY WEB SITE