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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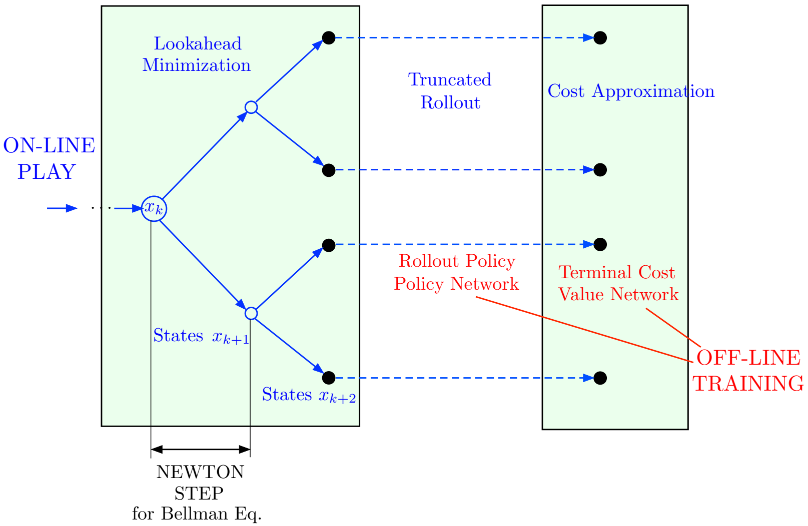
Lecture 11

We transition from on-line play to off-line training algorithms

Neural Nets, and Other Parametric Architectures

Outline

The AlphaZero/MPC Model: Our Starting Point



What We Have Done So Far

We started with four overview/big picture lectures (Chapter 1 of class notes)

- Off-line training, on-line play, Newton step interpretations
- Exact DP, deterministic, stochastic, finite and infinite horizon
- Approximation in value space and rollout
- Problem relations and transformations: State augmentations, termination state problems (e.g., stochastic shortest path), multiagent, POMDP
- Adaptive and model predictive control

Then focused at on-line play algorithms (Chapter 2 of class notes)

- Rollout algorithms for deterministic and stochastic problems; variations (fortified, simplified, constrained, model-free, variance reduction ideas)
- Multistep lookahead search for deterministic problems (pruning, double rollout)
- Multistep lookahead for stochastic problems (certainty equivalence approximations, Monte Carlo tree search)
- Multiagent/multicomponent control problems; variations (autonomous w/ signaling)
- Bayesian optimization, sequential estimation, adaptive control, and rollout

Where We Are Going and What is Left Out

Our plan for the next two lectures (Chapter 3 of class notes)

We will cover in some depth and detail

- Approximation of values and policies using neural nets and other architectures
- Training of approximation architectures with incremental gradient methods
- Approximate value and policy iteration with approximation architectures
- Aggregation

The 2019-2021 course videolectures, the 2019 RL book, and the 2012/2017 DP book deal with additional topics:

- More on the theory of infinite horizon problems
- Stochastic training methods for approximation in value space: TD(Lambda), other TD methods for policy evaluation, Q-learning
- Specialized methods for approximation in policy space: policy gradient methods, random search methods

Recall Approximation in Value Space for On-Line Control Selection

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 w/ approximations

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

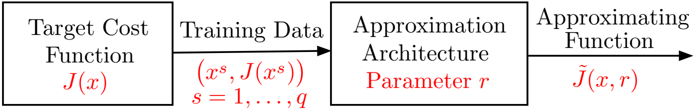
Off-Line Training: Types of Approximations

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

- Cost approximation in finite and infinite horizon problems
  - Optimal 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
  - Approximation of an optimal policy $\mu_k^*(x_k)$ or $\mu^*(x)$
  - Approximation of 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)



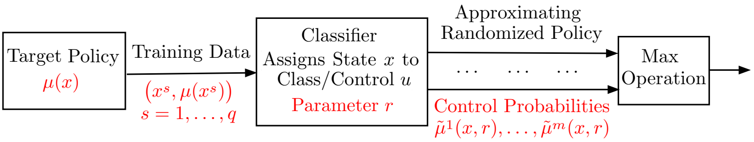
TRAINING CAN BE DONE WITH SPECIALIZED OPTIMIZATION SOFTWARE

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 $\{u^1, \ldots, u^m\}$, an alternative approach is possible and is commonly used
- View a policy μ as a classifier: A function that maps x into a “category" $\mu(x)$
- Some classifiers introduce randomized policies
- Then the output of the classifier is “control probabilities"



TRAINING CAN BE DONE WITH CLASSIFICATION SOFTWARE

Randomized policies have continuous components

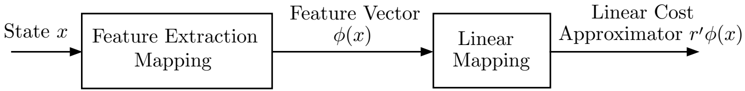
This helps algorithmically

Cost Function Parametric Approximation Generalities

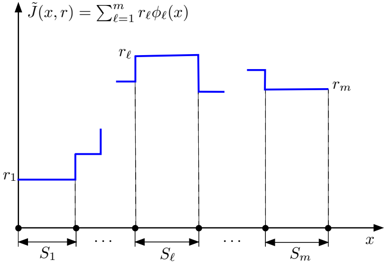
- We start with a class of functions $\tilde{J}(x, r)$ that depend on x and on a vector $r = (r_1, \ldots, r_m)$ of m "tunable" scalar parameters.
- We adjust r to change $\tilde{J}$ and "match" the training data from the target function.
- The training algorithm is the algorithm that chooses r (typically regression-type).
- 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 $\phi(x)$.



A Simple Example of a Linear Feature-Based Architecture



Piecewise constant approximation

- Partition the state space into subsets $S_1, \ldots, S_m$. The ℓth feature is 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

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

is piecewise constant with value r_ℓ for all x within the set S_ℓ.

Generic Polynomial Architectures

Quadratic polynomial approximation

- Let $x = (x^1, \dots, x^n)$
- 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

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

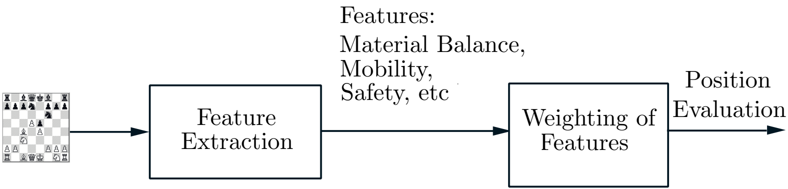
- Here the parameter vector r has components r_0, r_i, and r_{ij}.

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

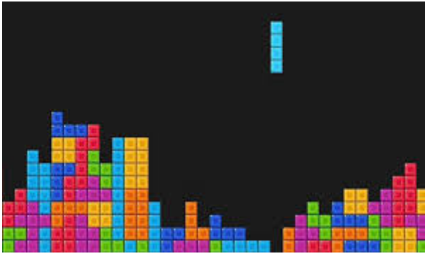
An even more general architecture: Polynomials of features of x

A linear feature-based architecture is a special case

Examples of Problem-Specific Feature-Based Architectures

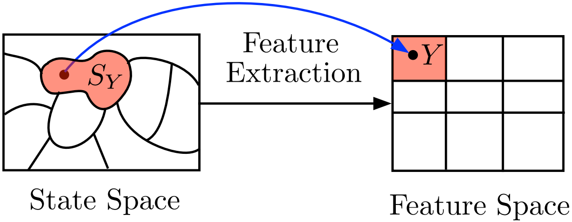


Chess



Tetris

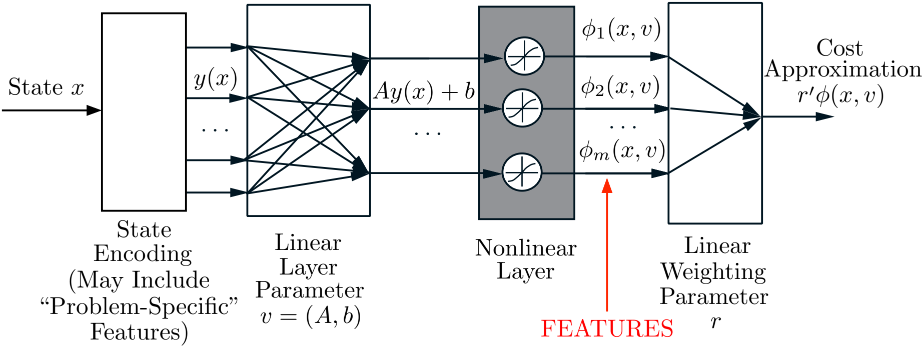
Architectures with Partitioned State Space



A simple method to construct complex approximation architectures:

- Partition the state space into several subsets and construct a separate cost approximation in each subset.
- 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
  - A manifestation of this idea arises in feature-based aggregation (next lecture)

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), $s = 1, \ldots, q$, where β^s is equal to the target cost $J(x^s)$ plus some "noise".
- r is determined by solving the problem

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

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

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 involves quadratic minimization 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 $\left(\tilde J(x^s, r) - \beta^s\right)^2$ at each iteration have worked well enough (for many problems).

Incremental Gradient Methods (Invented in the 80s, and Analyzed/Extended in the 90s to the Present)

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

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

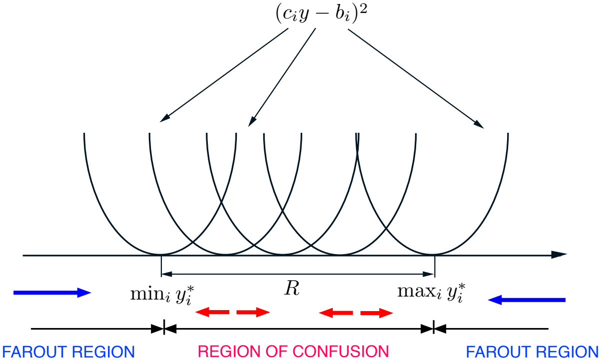
where $\gamma^k > 0$ is a stepsize parameter.

The incremental gradient counterpart

Choose an index i_k and iterate according to

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

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.

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

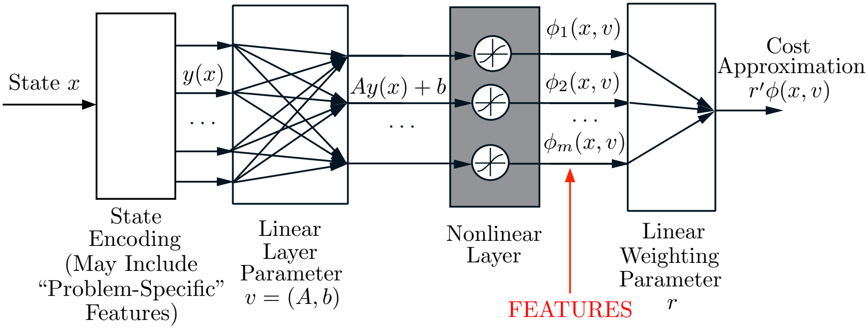
$$y^{k+1} = y^k - \gamma^k \nabla_y F(y^k, w^k)$$

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 class notes and references therein).

Neural Nets: An Architecture that Automatically Constructs Features

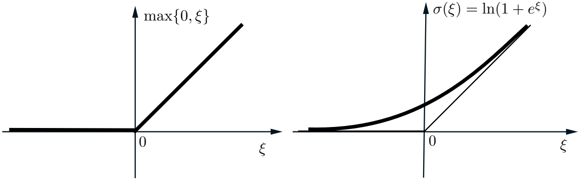


Given a set of state-cost training pairs (x^s, β^s), $s = 1, \ldots, q$, the parameters of the neural network (A, b, r) are obtained by solving the training problem

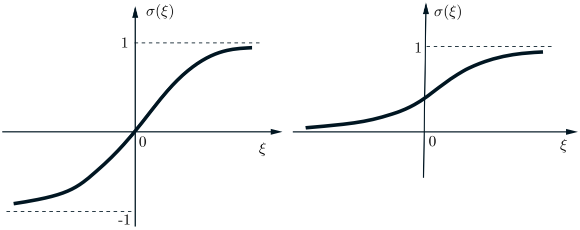
$$\min_{A,b,r} \sum_{s=1}^{q} \left(\sum_{\ell=1}^{m} r_\ell \sigma \left(\left(Ay(x^s) + b \right)_\ell \right) - \beta^s \right)^2$$

- Incremental gradient is typically used for training.
- Universal approximation property (can approximate "any" target function, arbitrarily well, with sufficiently large network size).

Rectifier and Sigmoidal Nonlinearities

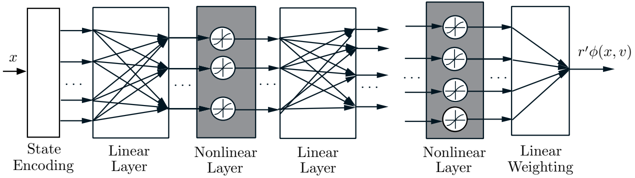


The rectified linear unit (ReLU) $\sigma(\xi) = \ln(1 + e^{\xi})$. It is the function $\max\{0, \xi\}$ with its corner "smoothed out."



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.

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

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

  affects the quality of the trained architecture (overparametrization if $R > 1$).
- 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 extensive research literature.

About the Next Lecture

We will cover:

- Value and policy iteration using neural networks
- Introduction to aggregation