Optimization-Based Approximate Dynamic Programming

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Thesis Objectives

- Reinforcement learning
 - Combines optimization and machine learning
- Challenge: Existing methods are unreliable

 Hard to use, analyze, and trust
- **Objective:** Develop more reliable methods that:
 - Provide better guarantees
 - Are easier to use, analyze, understand

• My approach:

- 1. Deepen understanding of basic principles
- 2. Build algorithms based on the basic principles

Application: Managing River Dam



Application: Managing Blood Inventories

- Managing blood inventory
 - Minimize shortage demand that is not satisfied
 - Maximize utilization –use before it perishes
- Take advantage of bloodtype compatibility



Domain Model

- Markov Decision Process
 States (grid) S
 - Actions: \mathcal{A}
- Optimal value function best utility of being in each state
- Optimal policy decision each state
- Optimal state visitation frequencies – how much time in each state



Maximize rewards Infinite horizon: discount: γ

Value Function and Policy

- True solution: policy
- Calculate policy π from VF v– Take the best greedy action
- Calculate VF for policy v_{π} – Add rewards for policy
- Policy visitation frequencies
 - How much time policy spends in a state $\,\,oldsymbol{\mathcal{U}}_{oldsymbol{\pi}}$
 - Upper bound (importance of a state) \mathcal{U}_{π}



Approximate Value Function

- Too large must approximate
- Value function based on state features

- = 1 - = 4

- Linear value function approximation
- **Representable** value functions



Restrict The Space of Value Functions

Small number of features

• Value function represented a small number of features

L₁ Regularization

- Large number of features
- Small volume

 $\tilde{v} = \Phi \times x$ $\tilde{v} = \Phi \times x$

Representable value functions

$$\mathcal{M} = \{ \mathbf{v} = \Phi x \, | \, \|x\|_{1,e} \le \psi \}$$

Value Function Approximation: Objectives

- How good is a policy π ?
- Expected policy loss $|v^*|$
- **Robust** policy loss $\|v^* v_{\pi}\|_{\infty}$
- How good is a value function v? – Quality of a greedy policy π
- Desirable bounds: for some *C*

$$\|v^* - v_{\pi}\|_{1,\alpha} \leq c \min_{v \in \mathcal{M}} \|v^* - v\|_{\infty}$$

Optimal

value function

Initial

distribution

Components of Value Function Approximation





Objectives

- If solved a problem using RL then patent it [Powell 2007]
- Major challenge: Off-the-shelf methods that are easy to use by non-practitioners
- I propose algorithms guided by error bounds
 - Strong guarantees & easy analysis
 - Good practical performance
- Easier to use, because we know:
 - When they work
 - Why they do not work

Why Is It Difficult?

- Many components must interact; balance errors:
 - Representational error: Due to features
 - Sampling error: Due to missing samples
 - Algorithmic error: Due to approximate optimization
- Better understand components to understand interaction



My Approach *

Classical Iterative Algorithms



Optimization-based algorithms



Approximate Dynamic Programming = Value Function Approximation

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Main Contributions

- Bottom-up: From simple to complex
- New and improved methods for
 1. Tight online error bounds
 - 2. VFA algorithms with strong guarantees
 - 3. Evaluating sample quality
 - 4. Automatically selecting features



Outline

1. Framework

Value function approximation

2. Optimization-based Formulations Approximate linear and bilinear programming

3. Sampling Bounds How good are samples

4. Feature Selection How to select good features





FRAMEWORK AND ITERATIVE ALGORITHMS

Bellman Operator L

• Propagates the expected value backwards

- Transition probabilities 0.5



• Bellman residual v - Lv

- BR: | 8 - (0.5*10+0.5*20) | = |8 - 15| = 7

- Measures self-consistency of the value function

Online Error Bounds: **Robust** Policy Loss



Online Error Bounds: Expected Policy Loss *



Online Error Bounds: Expected Policy Loss (Distribution) *



Approximate Policy Iteration

- Difficulty: Bellman operator is **nonlinear**
- API: Classical iterative VFA algorithm



- Bellman operator is linear for a fixed policy
- Based on *policy iteration*

Approximate Policy Iteration

- No convergence guarantees
- Do not know when to stop



Iteration

Offline Bounds for API *

Approximation Error Bounds

$$\limsup_{k \to \infty} \|v^* - v_{\pi^k}\|_{\infty} \leq \frac{2}{(1-\gamma)^3} \limsup_{k \to \infty} \|\tilde{v}_k - L\tilde{v}_k\|_{\infty}$$

- No convergence
- Large constants $\gamma = 0.99 \quad \frac{1}{1-\gamma} = 100 \quad \frac{1}{(1-\gamma)^3} = 1000000$ - Possibly larger than value function

$$\limsup_{k \to \infty} \|v^* - v_{\pi^k}\|_{\infty} > c\min_{v \in \mathcal{M}} \|v - v^*\|_{\infty}$$
 Desirable bound



OPTIMIZATION-BASED FORMULATIONS

Main Idea

Minimize online bounds – the bounds should be as tight as possible



For now assume that all samples are known

Approximate Linear Programming

- Classical approximation method
- Formulation
 - Constraints: transitions
 - Variables: features
- Guaranteed to converge
- Usually based on LP for MDPs



Bellman constraints

Approximate Linear Programming as an Optimization-based Method *

- LP to minimize online error bounds
- Robust policy loss cannot be LP (P<NP)

$$\|v^* - v_{\pi}\|_{\infty} \leq \frac{1}{1-\gamma} \|L\widetilde{v} - \widetilde{v}\|_{\infty}$$

• Expected policy loss as LP

$$\|v^* - v_{\pi}\|_{1,\alpha} \leq \alpha^{\mathsf{T}}(v^* - \tilde{v}) + \bar{u}_{\pi}^{\mathsf{T}} [\tilde{v} - L\tilde{v}]_+$$

– Easy to formulate as an LP when \overline{u}_{π} is fixed

– Visitation frequencies $ar{u}_\pi$ depend on $ar{v}$

ALP: Offline Error Bounds *

 Bound for opt-basedALP $\|v^* - v_{\pi}\|_{1,\alpha} \leq \frac{2\overline{u}_{\pi}^{\mathsf{T}} 1}{1 - \gamma} \min_{v \in \mathcal{M}} \|v^* - v\|_{\infty}$ $\propto \frac{2}{(1-\gamma)^2} \min_{v \in \mathcal{M}} \|v^* - v\|_{\infty}$ • Good value of \overline{u}_{π} is often unknown - Bound approximate value function $\|v^* - \tilde{v}\|_{1,c} \le \frac{2}{1-\gamma} \min_{v \in M} \|v^* - v\|_{\infty}$

Closest approximation

ALP: Practical Performance *

• Applied to blood inventory management



RALP: Alternative Formulation*

- Minimize a tighter **online** bound $\min_{\boldsymbol{v}\in\mathcal{M}} \left(\overline{\boldsymbol{u}}^{\mathsf{T}} (\mathbf{I} - \gamma P^*) - \alpha^{\mathsf{T}} \right) (\tilde{\boldsymbol{v}} - \boldsymbol{v}^*) + \overline{\boldsymbol{u}}^{\mathsf{T}} [L\boldsymbol{v} - \boldsymbol{v}]_+$
- Linear program:



• Offline error bound

$$\|v^* - v_{\pi}\|_{1,lpha} \propto rac{1}{1-\gamma} \min_{oldsymbol{v} \in \mathcal{M}} \|oldsymbol{v} - v^*\|_{\infty}$$

Does not depend on: $1/(1-\gamma)^2$

Approximate Linear Programming

- RALP: good performance
- Alternatives necessary

 Bounds are loose
 - Needs prior knowledge
- $\|v^* v_{\pi}\|_{1,\alpha} \leq \ldots + \overline{u}_{\pi}^{\mathsf{T}} [\widetilde{v} L\widetilde{v}]_{+}$
 - Often does not work
 - Why use ALP?
 - Easy to solve & analyze
 - Sometimes works well



Blood inventory management

Approximate Bilinear Programming

• Approximate policy iteration

• Approximate linear program

• Approximate bilinear program





Approximate Bilinear Programming: Derivation *

- Formulations for *all* online error bounds
- *Robust* policy loss

$$\|v^* - v_{\pi}\|_{\infty} \leq rac{1}{1 - \gamma} \| ilde{v} - L ilde{v}\|_{\infty}$$

• Expected policy loss (no prior knowledge)

$$\|v^* - v_{\pi}\|_{1,\alpha} \leq \alpha^{\mathsf{T}}(v^* - \tilde{v}) + \frac{1}{1 - \gamma} \|\tilde{v} - L\tilde{v}\|_{\infty}$$

• Expected policy loss (prior knowledge) $\|v^* - v_{\pi}\|_{1,\alpha} \leq \alpha^{\mathsf{T}}(v^* - \tilde{v}) + \bar{u}_{\pi}^{\mathsf{T}} [\tilde{v} - L\tilde{v}]_+$

Approximate Bilinear Programming *



ABP: Offline Error Bounds *

• Approximate Bilinear Programming

$$\|v_{\pi} - v^*\|_{\infty} \leq \frac{2}{1 - \gamma v \in \mathcal{M}} \|Lv - v\|_{\infty}$$

• Approximate Linear Programming

$$\|v_{\pi} - v^*\|_{\infty} \leq \frac{(2+\gamma)|\mathcal{S}|}{(1-\gamma)^2} \min_{v \in \mathcal{M}} \|v^* - v\|_{\infty}$$

• Approximate Policy Iteration

$$\limsup_{k \to \infty} \|v_{\pi^k} - v^*\|_{\infty} \leq \frac{2}{(1 - \gamma)^2} \limsup_{k \to \infty} \|\tilde{v}_k - v_k\|_{\infty}$$
Solving Approximate Bilinear Programs

- Value function approximation is NP hard
- Simple approximate algorithm



Approximate Bilinear Programming

- **ABP** Guarantees •
 - Tight value function approximation
 - Convergence
 - Match performance of API
- ABP, ALP works well in •
 - Benchmark problems
 - Reservoir management
- Opportunity for better
 - Algorithms
 - Analysis











Expected Policy Loss

Robust Policy Loss



SAMPLING ERROR

Solution Based On Samples

- Problems with many states
- Reservoir management

 State = water level
 State = water level



- Would have solve the problem for **all** water levels
- ALP: One constraint per state
- Challenge: Bound policy loss due to sampling
- No practical bounds exist

- Too loose or impossible to compute

Types Of Sampling Error

State selection error

• States that are not sampled



Transition estimation error

• States that are sampled, but are not known precisely



Bounding Sampling Error *

- **Approach:** Bounds using the simple analysis of optimization-based VFA
- Regularized representable value functions $\mathcal{M} = \{ \mathbf{v} = \Phi x \, | \, \|x\|_{1,e} \leq \psi \}$
- $\epsilon_p(\psi)$ State selection error: how different are unsampled states
- $\epsilon_s(\psi)$ Transition estimation error: how different are state transitions from the true value

Sampling: Offline Error Bounds *

Bounds on policy loss

$$-\operatorname{ALP}_{\|\tilde{v}-v^*\|_{1,c} \leq \frac{2}{1-\gamma v \in \mathcal{M}} \|v-v^*\|_{\infty} + 2\epsilon_c(\psi) + \frac{3\epsilon_s(\psi) + 2\epsilon_p(\psi)}{1-\gamma} - \operatorname{ABP}_{\|\tilde{v}-L\tilde{v}\|_{\infty} \leq \min_{v \in \mathcal{M}} \|v-Lv\|_{\infty} + 2\epsilon_s(\psi) + \epsilon_p(\psi)}$$

 Assumptions too general to be useful directly – How to estimate them?

State Selection Error: Local Modeling Assumption

- States that are close are similar
- Seen a Lipschitz continuity



Basic Approach *

- How to use that samples are known?
- Map the states to samples $\chi: \mathcal{S} \to \Sigma$



Problems with Local Modeling

Assumption must apply to the full state space

- Bounds are too loose to be useful

 Functions tend to be constant with small discountinuities



• Hard to estimate the similarity

Better Bounds *

- Use the global structure of the problem
- Usually more than a single sample available
- Map a state to multiple samples



 Linear segments do not incur any error Rewarc

Bayesian Regression Assumption *

- Local modeling:
 - Worst-case guarantees: pessimistic assumptions
 - Local analysis
- Use Bayesian regression to generalize to unsampled states
 - Take advantage of global structure
 - Expectation instead of hard bounds easy to specify
- Drawback:
 - Probabilistic guarantees

Comparison To Local Modeling *

- Gaussian processes
- Tight bounds (10-100x tighter than LM)
- Flexible assumptions
- Can be used in practice



Transition Estimation Error *

- Offline error bound $\mathbf{P}\left[\epsilon_{s}(\psi) > \epsilon\right] \leq 2|\tilde{\boldsymbol{\Sigma}}|_{a}|\phi| \exp\left(\frac{2(\epsilon/(\psi \cdot \gamma))^{2}}{M_{\phi}n}\right)$
- Depends on the number of samples $|\tilde{\Sigma}|_a$
- The bound is tight
- Need many weather patterns need to be sampled per volume



Common Random Numbers

• The bounds are tight because state are estimated independently

 Idea: Use the same weather to evaluate every volume



Common Random Numbers *

• Growth function $\tau(m)$

- How similar is behavior for all kinds of volumes

$$\mathbf{P}\left[\epsilon_{s}(\psi) > \epsilon\right] \leq 2|\phi| \exp\left(\frac{2(\epsilon/(\psi \cdot \gamma \cdot |\boldsymbol{\tau}(\boldsymbol{m})|))^{2}}{M_{\phi}m}\right)$$

- Independent of number of samples
- Similar concept to VC dimension



Sampling Error

• Approximate Policy Iteration [Farahmand et al. 2009]

$$\limsup_{n \to \infty} \|v^* - v_n\|_{\infty} \leq \limsup_{n \to \infty} \frac{2\gamma}{(1 - \gamma)^2} \left(c \times C_{\rho,\nu} \max_{i \leq n} \|\epsilon_i\|_{\rho,\nu} + \ldots \right)$$

Theoretically interesting

- Hard/impossible to use in practice
- Approximate Bilinear Programming

 $\|\tilde{v} - L\tilde{v}\|_{\infty} \leq \min_{v \in \mathcal{M}} \|v - Lv\|_{\infty} + 2\epsilon_s(\psi) + \epsilon_p(\psi)$

- Easy to use general properties
- Can be used in practice (limited)



FEATURE SELECTION

Choosing Features

- Must approximate the value function
- Need a small number of features
 - Optimization problems easy to solve
 - Minimizes sampling error

Features are hard to choose

Must know which states are important
 Possible binary features in reservoir management:

 $l \in [1,6] \ l \in [7,10] \ l \in [3,12] \ l \in [10,15]$. .





Number of Features and Solution Quality *



Automatically choose features based on sampling bounds

Selecting Features To Balance Errors*



- Determine the global minimum
 - Homotopy method: efficiently calculate the solution for all values of ψ

Automatic Feature Selection ALP



Feature Selection

- When sampling bounds available
 Can select appropriate features/regularization
- Performance does not decrease with more features
 - Flexibility in specifying features
- Outperforms other algorithms in benchmark problems

CONCLUSION

Conclusion

- Iterative algorithms have weak guarantees
 - Unreliable
 - Hard to analyze
- New & improved optimization-based algorithms
 - Decouple objective from algorithm
 - Strong guarantees
 - Easy to analyze and use
- (More) Practical sampling bounds: Use Gaussian processes
- Feature selection: Balance feature complexity with samples

Algorithms for Value Function Approximation

Classical Iterative Algorithms

• Based on MDP algorithms

- Simple algorithms
- Complex analysis
 - Weak guarantees
 - Hard to analyze
 - Hard to use

Optimization-based Algorithms

- Based on value-function bounds
- More complex algorithms
- Simple analysis
 - Strong guarantees
 - Sampling bounds
 - Feature selection

Contributions

- Analysis of API [NIPSO8, ECML/ML09]
- New, robust VFA formulations [ICAPSO8]
 - ALP: new derivation and formulation [ICML09]
 - ABP: robust/expected policy loss [NIPSO9,JMLR?]
- Sampling bounds and feature selection
 - New better sampling bounds [ICML10,NIPS?]
 - Methods for feature selection [IJCAI07,ICML10]
- Mathematical optimization algorithms
 - Homotopy methods [ICML10]
 - Bilinear program solvers [AAAI07, JAIR09]



APPENDIX

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MATHEMATICAL OPTIMIZATION ALGORITHMS

Algorithmic Considerations

- Optimization-based formulation require solving optimization problems
- Approximate linear programs
 - Solving large linear programs
 - Mature solvers that can solve large problems
- Approximate bilinear programs
 - NP hard to solve optimally
 - Few solvers are available

Solving Approximate Linear Programs

 Small number of features minimize Easy to solve subject to * Large number of features minimize Harder to solve subject to * Homotopy Methods for Approximate Linear Programs *

• Solve for large ALPs with **regularization**



Important: Address degenerate solutions – dual regularization

$$\max_{\substack{y,\lambda\\y,\lambda}} b^{\mathsf{T}}y - \psi\lambda + \frac{1}{\chi}y^{\mathsf{T}}y$$

s.t. $A^{\mathsf{T}}y - e\lambda \leq c$
 $y,\lambda > 0$

$$\min_{x} c^{\mathsf{T}}x + \chi \frac{1}{2} \left\| [Ax - b]_{+} \right\|_{2}^{2}$$
s.t. $e^{\mathsf{T}}x \le \psi$
 $x \ge 0$

Solving Bilinear Programs

- Few bilinear program solvers
- Easier to solve when the number of bilinear terms is small
 - Method for solving such BPs (*)
- An instance of a global optimization problem
 - Concave quadratic minimization
 - Mixed integer linear program
- Commercial solvers available

Standard MILP Transformation

$$\begin{array}{ll} \min_{\substack{w,\lambda_1,z,\lambda_2,q_1,q_2 \\ \text{s.t.}}} & s_2^{\mathsf{T}} z + \lambda_1^{\mathsf{T}} b_1 \\ & A_1 A_2^{\mathsf{T}} \lambda_2 - A_1 r_2 + B_1 w \ge b_1 \\ & A_1 A_2^{\mathsf{T}} \lambda_2 - A_1 r_2 + B_1 w \ge b_1 \\ & A_1^{\mathsf{T}} \lambda_1 = r_1 + C y \\ & B_1^{\mathsf{T}} \lambda_1 = s_1 \\ & B_1^{\mathsf{T}} \lambda_1 = s_1 \\ & A_1 A_2^{\mathsf{T}} \lambda_2 - A_1 r_2 + B_1 w - b_1 \le (1 - q_1) M \\ & A_2 A_1^{\mathsf{T}} \lambda_1 - A_2 r_1 + B_2 z - b_2 \le (1 - q_2) M \\ & \lambda_1 \le M q_1 \\ & \lambda_1 \ge 0 \\ & q_1 \in \{0, 1\}^n \\ \end{array}$$

- Hard to analyze
- MILP solvers work very poorly

MILP Formulation of ABP *

$$\min_{\substack{z,\pi,\lambda,\lambda',\nu\\\text{s.t.}}} \mathbf{1}^{\mathsf{T}}z + \lambda'$$

$$z \ge \lambda - (\tau - \pi)$$

$$\lambda + \lambda' \mathbf{1} \ge Av - b$$

$$Av - b \ge \mathbf{0}$$

$$B\pi = \mathbf{1} \quad \lambda, \lambda' \ge \mathbf{0}$$

$$v \in \mathcal{M} \quad \pi \in \{0,1\}^n$$
• Corders of magnitude faster to solve

• Still not fast enough
OTHER SLIDES

Types of Algorithm

- **Policy based**: *policy search*
 - Does not explicitly use a value function
 - Great results, but hard to analyze
- Value function based: approximate dynamic programming
 - Calculate value function as an intermediate step
 - Stronger guarantees, good performance

All efficient methods for sequential decision problems estimate value function as an intermediate step.

Richard Sutton, MSRL 2009

Lower Bounds on API Performance *

• A trivial bound can be tighter for sufficiently high discount factors

$$\limsup_{k \to \infty} \|v^* - v_{\pi^k}\|_{\infty} \leq \frac{c}{1 - \gamma} < \frac{2}{(1 - \gamma)^3} \limsup_{k \to \infty} \|\tilde{v}_k - L\tilde{v}_k\|_{\infty}$$

Impossible to get bounds in terms of the best approximation

$$\limsup_{k \to \infty} \|v^* - v_{\pi^k}\|_{\infty} > c \min_{v \in \mathcal{M}} \|v - Lv\|_{\infty}$$

Algorithms for VF Approximation

- Combines features and samples
- Resembles machine learning regression





Relationship To Machine Learning

- No distribution in regression
- Distribution depends on the policy
 policy depends on the value function
- The guarantees must be different

Value Function Approximation





The Bound Is Tight *



Modify ALP to reduce the bound

Improve practical performance

Why Approximation Fails? *

• Virtual Loop



Expanding Constraints *

Roll out selected constraints
Use dual values

• Offline error bounds

$$\|\tilde{v}_{t} - v^{*}\|_{1} \leq \frac{2}{1 - \gamma^{t}} \min_{v \in \mathcal{M}} \|v^{*} - v\|_{\infty}$$
$$\gamma = 0.99 \ \frac{1}{1 - \gamma} = 100 \ t = 10 \ \frac{1}{1 - \gamma^{t}} = 10.5$$



Simple Approximate Algorithm for ABP

- Motivates approximate policy iteration
- Converges



Automatic Feature Selection ABP

- ALP relies on convexity
- ABP is NOT convex

– But can use a similar property



Future Work: Modeling

- Data is used directly
 - Not enough data
 - Incorporating prior knowledge?

- Interaction of models and optimization
 - Integrate machine learning components

Future Work: Optimization-based Algorithms

- Optimization-based ADP methods in practice
 - Performance?
 - What is a good value function?
 - Implications for iterative algorithms?

- Algorithms for linear/bilinear programs
- Tighter bounds
 - Better ways to samples