

Stable Models and Temporal Difference Learning

Gaurav Manek

CMU-CS-23-103

March 2023

School of Computer Science
Carnegie Mellon University
Pittsburgh, PA 15213

Thesis Committee:

J. Zico Kolter, Chair

David Held

Deepak Pathak

Sergey Levine (Berkeley)

*Submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy.*

Copyright © 2023 Gaurav Manek

This research was sponsored by A*STAR Graduate Academy, Robert Bosch GmbH, and the NSS Fellowship.

The views and conclusions contained in this document are those of the author and should not be interpreted as representing the official policies, either expressed or implied, of any sponsoring institution, the U.S. government or any other entity.

March 9, 2023
DRAFT

Keywords: Lyapunov Stability, Regularization, Deadly Triad, Offline Reinforcement Learning, Temporal Difference Learning, Reinforcement Learning, Neural Networks, Machine Learning Theory

March 9, 2023
DRAFT

Abstract

In this thesis, we investigate two different aspects of stability: the stability of neural network dynamics models and the stability of reinforcement learning algorithms. In the first chapter, we propose a new method for learning Lyapunov-stable dynamical models that is stable by construction, even when randomly initialized. We demonstrate the effectiveness of this method on damped multi-link pendulums and show how it can be used to generate high-fidelity video textures.

In the second and third chapters, we focus on stability issues in reinforcement learning. In the second chapter, we demonstrate that regularization, a common approach to addressing instability in temporal difference (TD) learning, is not always effective. We show that TD learning can diverge even when regularization is used and demonstrate this phenomenon in standard examples as well as a novel problem we construct.

In the third chapter, we propose a new resampling strategy called Projected Off-Policy TD (POP-TD), which resamples TD updates to come from a convex subset of “safe” distributions. Unlike existing resampling methods, it need not converge to the on-policy distribution. We show how this approach can mitigate the distribution shift problem in offline RL on a task designed to maximize such shift.

Overall, this thesis advances novel methods for dynamics model stability and training stability in reinforcement learning, questions existing assumptions in the field, and points to promising directions for stability in model and reinforcement learning.

Contents

Introduction	vii
1 Learning Stable Dynamics Models	1
1.1 Introduction	2
1.2 Background and related work	3
1.3 Joint learning of dynamics and Lyapunov functions	6
1.3.1 Properties of the Lyapunov function	7
1.4 Empirical results	11
1.4.1 Random networks	12
1.4.2 n-link pendulum	12
1.4.3 Video Texture Generation	13
1.5 Conclusion	16
1.6 Adaptation to Stable Control and RL	16
2 The Pitfalls of Regularization in Off-Policy TD	19
2.1 Introduction	21
2.2 Preliminaries and Notation	25
2.3 Our Counterexamples	26
2.3.1 Regularization cannot always mitigate off-policy training error.	27
2.3.2 Small amounts of regularization can cause large increases in training error.	34
2.3.3 Emphatic approaches and our counterexample	36

2.3.4	Applied to multi-layer networks	46
2.3.5	Over-parameterization does not solve this problem	47
2.4	Related Work	49
2.5	Relationship to modern RL algorithms	50
2.6	Conclusion	50
3	Projected Off-Policy TD for Offline Reinforcement Learning	55
3.1	Introduction	56
3.2	Related Work	57
3.3	Problem Setting and Notation	59
3.3.1	The Non-Expansion Criterion (NEC)	60
3.4	Projected Off-Policy TD (POP-TD)	62
3.4.1	I- and M-projections	63
3.4.2	Optimizing the distribution	63
3.4.3	The structure of Z	64
3.4.4	Update rules	66
3.4.5	POP-Q-Learning	67
3.5	Experiments and Discussion	69
3.5.1	POP-Q on GridWorld	70
3.5.2	Linear POP-Q on GridWorld	72
3.6	Conclusion	73
	Conclusion	79
	Notation and Definitions	81
	Bibliography	82

1 Introduction

2 In this thesis we examine two notions of stability: the predictions of neural network
3 dynamics models and the training of reinforcement learning algorithms. The transition
4 from the first notion of stability to the second is natural: the parameters of a stably
5 trained model circumscribes, in parameter-space, a stable trajectory. This relationship
6 between stabilities has significant precedence in the foundational work of Temporal
7 Difference (TD) learning theory [53].

8 In the first chapter we propose a new method for learning Lyapunov-stable dynamical
9 models and the certifying Lyapunov function in a fully end-to-end manner. This
10 works by carefully constructing a neural network to act as a Lyapunov function and
11 learning a separate, unconstrained model. These two models are combined with a
12 novel reprojection layer to produce models that are guaranteed stable by construction,
13 even without any training. We show that such learning systems are able to model
14 simple dynamical systems such as pendulums, and can be combined with additional
15 deep generative models to learn complex dynamics, such as video textures, in a fully
16 end-to-end fashion, given Temporal Difference (TD) data.

17 Next, we attempted to extend this work to learn control policies that produce stable
18 trajectories. This is a natural extension of the previous work, equivalent to only
19 minor changes to the construction of the dynamics model. Our work necessarily
20 learned from TD data collected by a different policy (i.e. offline). Despite immense
21 effort and many experiments, this technique never converged to reasonable solutions,
22 even with regularization. This led to the insights in the second chapter.

23 TD is combined with function approximation (i.e. neural networks) and off-policy
24 learning in modern Reinforcement Learning. However, these three ingredients are
25 known as the *deadly triad* [48, p. 264], because they are known to cause severe
26 instability in the learning process Tsitsiklis and Van Roy [53]. While many variants of
27 TD will provably converge despite the training instability, the quality of the solution
28 at convergence is typically arbitrarily poor [24]. In the literature, there is a general
29 belief that regularization can mitigate this instability, which is supported by basic
30 analysis on the three standard examples.

31 However, this is not true! In the second chapter, we introduce a series of new
32 counterexamples that are resistant to regularization. We demonstrate the existence
33 of “vacuous” examples, which never do better than the limiting case regardless of the
34 amount of regularization. This problem persists in most TD-based algorithms, which
35 covers a wide swath of the RL literature; we make our analysis concrete by showing
36 how this example forces the error bounds derived by Zhang, Yao, and Whiteson
37 [62] to permit vacuous solutions. We further demonstrate that regularization is not
38 monotonic in TD contexts, and that it is possible for regularization to increase error
39 (or cause divergence) around some critical values. We extend these examples to the
40 neural network case, showing that these effects are not limited to the linear case
41 and making the case for greater care in regularization in practical RL applications.
42 Finally, contemporary versions of Emphatic-TD generally use a reversed version of
43 TD to estimate the resampling function, which opens them up to instability from
44 the same source as the original TD. We show that these techniques are similarly
45 vulnerable. We show that regularization is not a panacea for stability in TD learning.

46 In the third chapter, we investigate new methods for stable TD learning that are
47 resistant to off-policy divergence and that do not rely on regularization. Starting
48 from previous work by Kolter [24], we derive Projected Off-Policy TD, which reweighs
49 TD updates to the closest distribution where the TD is non-expansive at the fixed
50 point of its training. We learn the reweighing factors in-the-loop with vanilla TD
51 methods (i.e. optimized as an augmented objective using stochastic gradient descent)
52 and then apply those reweighing factors to each TD update. Crucially, this is distinct

53 from contemporary work in the literature in that POP-TD does not resample to on-
54 policy distribution, instead finding a “safe” distribution close to the data distribution.
55 Applying this to a novel offline RL example, we can clearly demonstrate how POP-TD
56 mitigates the *distributional shift* between the dataset and the learned policy [30]
57 while resampling as little as possible.

58 We conclude with a discussion on future directions that our work on stable models
59 may take.

60 Chapter 1

61 Learning Provably Stable Deep 62 Dynamics Models

63 Deep networks are commonly used to model dynamical systems, predicting how the
64 state of a system will evolve over time (either autonomously or in response to control
65 inputs). Despite the predictive power of these systems, it has been difficult to make
66 formal claims about the basic properties of the learned systems. In this chapter,
67 we propose an approach for learning dynamical systems that are guaranteed to be
68 stable over the entire state space. The approach works by jointly learning a dynamics
69 model and Lyapunov function that guarantees non-expansiveness of the dynamics
70 under the learned Lyapunov function. These two models are combined with a novel
71 reprojection layer to produce models that are guaranteed stable by construction,
72 even without any training. We show that such learning systems are able to model
73 simple dynamical systems such as pendulums, and can be combined with additional
74 deep generative models to learn complex dynamics, such as video textures, in a fully
75 end-to-end fashion.

76 *From “Learning Stable Deep Dynamics Models” by Manek and Kolter (2019)*

77 1.1 Introduction

78 This chapter deals with the task of learning continuous-time dynamical systems.

79 Given $x(t) \in \mathbb{R}^n$, a state at time t , we wish to model the time-derivative

$$80 \quad \dot{x}(t) \equiv \frac{d}{dt}x(t) = f(x(t)) \quad (1.1)$$

81 for some function $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$. Modeling the time evolution of such dynamical
82 systems (or with control inputs $\dot{x}(t) = f(x(t), u(t))$ for $u(t) \in \mathbb{R}^m$) is a foundational
83 problem in machine learning, with applications in reinforcement learning, control,
84 forecasting, and many other settings. Owing to their representational power, neural
85 networks have long been a natural choice for modeling the function f [14, 41, 37, 12].
86 However, when using a generic neural network to model dynamics in this setting,
87 very little can be guaranteed about the behavior of the learned system, especially
88 about its *stability*. Informally, we say that a model is stable if we can pick a bounded
89 set of states and guarantee that once the model enters that set it never leaves. While
90 some recent work has begun to consider stability properties of neural networks [6, 45,
91 51], it has typically done so by softly enforcing stability as an additional loss term on
92 the training data. Consequently, they can say little about the stability of the system
93 in unseen states.

94 In this paper, we propose an approach to learning neural network dynamics that are
95 provably Lyapunov-stable over the entirety of the state space. We do this by jointly
96 learning a nominal system dynamics and the certifying Lyapunov function, and then
97 reproject the predictions of the nominal model onto the level set of the Lyapunov
98 function. This stability is a hard constraint imposed upon the model: unlike recent
99 approaches, we do not enforce stability via an imposed loss function but build it
100 directly into the dynamics of the model. This means that even a randomly initialized
101 model in our proposed model class will be provably stable everywhere in state space.
102 The key to this is the design of a proper Lyapunov function, based on input convex
103 neural networks [1], which ensures global exponential stability to an equilibrium point
104 while still allowing for expressive dynamics.

105 Using these methods, we demonstrate learning dynamics of physical models such as
 106 n -link pendulums, and show a substantial improvement over generic networks. We
 107 also show how such dynamics models can be integrated into larger network systems to
 108 learn dynamics over complex output spaces, combining the model with a variational
 109 auto-encoder (VAE) [23] to learn dynamic “video textures” [46].

110 1.2 Background and related work

111 **Stability of dynamical systems.** We consider the setting of uncontrolled dynamics
 112 systems $\dot{x}(t) = f(x(t))$ for $x(t) \in \mathbb{R}^n$. (We will discuss extending this to dynamics
 113 with control later; this is a non-trivial extension.) Such a system is defined to be
 114 *globally asymptotically stable* around the equilibrium point $x_e = 0$ if we have $x(t) \rightarrow 0$
 115 as $t \rightarrow \infty$ for any initial state $x(0) \in \mathbb{R}^n$; f is *locally asymptotically stable* if the
 116 same holds but only for $x(0) \in \mathcal{B}$ where \mathcal{B} is some bounded set containing the origin.
 117 Similarly, f is *globally* or *locally* exponentially stable if

$$118 \quad \|x(t)\|_2 \leq m \|x(0)\|_2 e^{-\alpha t} \quad (1.2)$$

119 for some constants $m, \alpha \geq 0$ for any $x(0) \in \mathbb{R}^n$ (\mathcal{B} , respectively).

120 The area of Lyapunov theory [20, 29] establishes the connection between the various
 121 types of stability mentioned above and descent according to a particular type of
 122 function known as a Lyapunov function. Specifically, let $V : \mathbb{R}^n \rightarrow \mathbb{R}$ be a continuously
 123 differentiable positive definite function, i.e., $V(x) > 0$ for $x \neq 0$ and $V(0) = 0$.
 124 Lyapunov analysis says that f is stable (according to the different definitions above),
 125 if and only if we can find some function V as above such the *value of this function is*
 126 *decreasing along trajectories generated by f* . Formally, this is the condition that the
 127 time derivative $\dot{V}(x(t)) < 0$, i.e.,

$$128 \quad \dot{V}(x(t)) \equiv \frac{d}{dt} V(x(t)) = \nabla V(x)^T \frac{d}{dt} x(t) = \nabla V(x)^T f(x(t)) < 0 \quad (1.3)$$

129 This condition must hold for all $x(t) \in \mathbb{R}^n$ or for all $x(t) \in \mathcal{B}$ to ensure global or local

130 stability respectively. Similarly f is globally asymptotically stable if and only if there
131 exists positive definite V such that

$$132 \quad \dot{V}(x(t)) \leq -\alpha V(x(t)), \quad \text{with } c_1 \|x\|_2^2 \leq V(x) \leq c_2 \|x\|_2^2. \quad (1.4)$$

133 Showing that these conditions imply the various forms of stability is relatively
134 straightforward, but showing the converse (that any stable system must obey this
135 property for some V) is relatively more complex. In this chapter we are largely
136 concerned with the “simpler” of these two directions, as our goal is to enforce
137 conditions that ensure stability.

138 **Stability of linear systems.** For a linear system with matrix A

$$139 \quad \dot{x}(t) = Ax(t) \quad (1.5)$$

140 it is well-known that the system is stable if and only if the real components of the
141 the eigenvalues of A are all strictly negative ($\text{Re}(\lambda_i(A)) < 0$). Equivalently, the same
142 same property can be shown via a positive definite quadratic Lyapunov function

$$143 \quad V(x) = x^T Q x \quad (1.6)$$

144 for $Q \succ 0$. In this case, by Equation 1.4, the following ensures stability:

$$145 \quad \dot{V}(x(t)) = x(t)^T A^T Q x(t) + x(t)^T Q A x(t) \leq -\alpha x(t)^T Q x(t) \quad (1.7)$$

146 i.e., if we can find a positive definite matrix $Q \succeq I$ with that $A^T Q + Q A + \alpha Q \preceq 0$
147 negative semidefinite. Such bounds (and much more complex extensions) for the
148 basis for using linear matrix inequalities (LMIs), as a method to ensure stability of
149 linear dynamical systems. The methods also have applicability to non-linear systems,
150 and several authors have used LMI analysis to learn non-linear dynamical systems by
151 constraining the linearized systems to have global Lyapunov functions [21, 2, 54],

152 Even though the constraints

$$153 \quad Q \succeq I, \quad A^T Q + Q A + \alpha Q \preceq 0 \quad (1.8)$$

154 are convex in A and Q separately, they are not convex in A and Q jointly. Thus, the
155 problem of jointly learning a stable linear dynamical system and its corresponding
156 Lyapunov function, even for the simple linear-quadratic setting, is *not* a convex
157 optimization problem, and alternative techniques such as alternating minimization
158 need to be employed instead. Past work has considered different heuristics, such as
159 approximately projecting a dynamics function A onto the (non-convex) stable set of
160 matrices with eigenvalues $\text{Re}(\lambda_i(A)) < 0$ [3]. It is no surprise, then, that learning
161 stable non-linear systems is even more challenging:

162 **Stability of non-linear systems** For general non-linear systems, establishing
163 stability via Lyapunov techniques is typically even more challenging. For the typical
164 task here, which is that of establishing stability of some *known* dynamics $\dot{x}(t) =$
165 $f(x(t))$, finding a suitable Lyapunov function is often more an art than a science.
166 Although some general techniques such as sum-of-squares certification [43, 42] provide
167 general methods for certifying stability of polynomial (or similar) systems, these are
168 often expensive and don't easily scale to high dimensional systems. Our proposed
169 approach here is able to learn provably stable systems without solving this (generally
170 hard) problem. Specifically, while it is difficult to find a Lyapunov function that
171 certifies the stability of some *known* system, we exploit the fact that it is relatively
172 much easier to *enforce* some function to behave in a stable manner according to a
173 Lyapunov function.

174 **Lyapunov functions in deep learning** Finally, there has been a small set of
175 recent work exploring the intersection of deep learning and Lyapunov analysis [6,
176 45, 51]. Although related to our work here, the approach in this past work is quite
177 different. As is more common in the control setting, these papers try to learn neural-
178 network-based Lyapunov functions for control policies, but in way that enforces

179 stability via a loss penalty. For instance Richards et al., [45] optimize a loss function
 180 that encourages $\dot{V}(x) \leq 0$ for x in some training set. In contrast, our work guarantees
 181 absolute stability *everywhere* in the state space, not just at a small set of points; but
 182 only for a simpler setting where the *entire* dynamics are to be learned (and hence can
 183 be “forced” to be stable) rather than a stabilizing controller for known dynamics.

184 1.3 Joint learning of dynamics and Lyapunov func- 185 tions

186 The intuition of the approach we propose in this paper is straightforward: instead
 187 of learning a dynamics function and attempting to separately verify its stability via
 188 a Lyapunov function, we propose to *jointly learn a dynamics model and Lyapunov*
 189 *function, where the dynamics is inherently constrained to be stable (everywhere in the*
 190 *state space) according to the Lyapunov function.*

191 Specifically, following the principles mentioned above, let $\hat{f} : \mathbb{R}^n \rightarrow \mathbb{R}^n$ denote a
 192 “nominal” dynamics model, and let $V : \mathbb{R}^n \rightarrow \mathbb{R}$ be a positive definite function:
 193 $V(x) \geq 0$ for $x \neq 0$ and $V(0) = 0$. Then in order to (provably, globally) ensure
 194 that a dynamics function is stable, we can simply project \hat{f} such that it satisfies the
 195 condition

$$196 \quad \nabla V(x)^T \hat{f}(x) \leq -\alpha V(x) \quad (1.9)$$

197 i.e., we define the dynamics

$$\begin{aligned}
 f(x) &= \text{Proj} \left(\hat{f}(x), \{f : \nabla V(x)^T f \leq -\alpha V(x)\} \right) \\
 &= \begin{cases} \hat{f}(x) & \text{if } \nabla V(x)^T \hat{f}(x) \leq -\alpha V(x) \\ \hat{f}(x) - \nabla V(x) \frac{\nabla V(x)^T \hat{f}(x) + \alpha V(x)}{\|\nabla V(x)\|_2^2} & \text{otherwise} \end{cases} \quad (1.10) \\
 &= \hat{f}(x) - \nabla V(x) \frac{\text{ReLU}(\nabla V(x)^T \hat{f}(x) + \alpha V(x))}{\|\nabla V(x)\|_2^2}
 \end{aligned}$$

Trajectory and Lyapunov function Case 1 Case 2

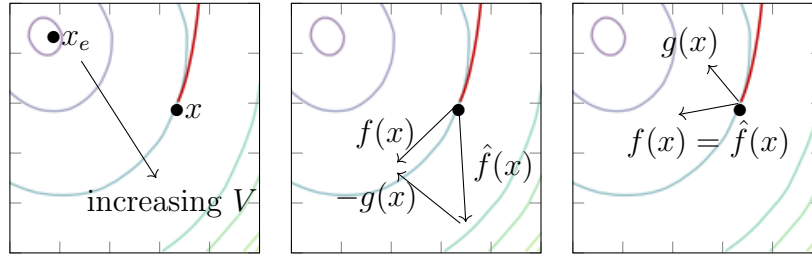


Figure 1.1: We plot the trajectory and the contour of a Lyapunov function of a stable dynamical system and illustrate our method. Let $g(x) = \frac{\nabla V(x)}{\|\nabla V(x)\|_2} \text{ReLU}(\nabla V(x)^T \hat{f}(x) + \alpha V(x))$. In the first case $\hat{f}(x)$ has a component $g(x)$ not in the half-space, which we subtract to obtain $f(x)$. In the second case $\hat{f}(x)$ is already in the half-space, so is returned unchanged.

199 where $\text{Proj}(x; \mathcal{C})$ denotes the orthogonal projection of x onto the point \mathcal{C} , and where
 200 the second equation follows from the analytical projection of a point onto a half-space.
 201 As long as V is defined using automatic differentiation tools, it is straightforward to
 202 include the gradient ∇V terms into the definition of f , and our final network can
 203 be trained just like any other function. The general approach here is illustrated in
 204 Figure 1.1.

205 1.3.1 Properties of the Lyapunov function V

206 Although the treatment above seems to make the problem of learning stable systems
 207 quite straightforward, the subtlety of the approach lies in the choice of the function
 208 V . Specifically, V needs to be positive definite and needs to have *no local optima*
 209 *except 0*. This is due to Lyapunov decrease condition: recall that we are attempting
 210 to guarantee stability to the equilibrium point $x = 0$, yet the decrease condition
 211 imposed upon the dynamics means that V is decreasing along trajectories of f . If V
 212 has a local optimum away from the origin, the dynamics can in theory get stuck in
 213 this location; this manifests itself by the $\|\nabla V(x)\|_2^2$ term going to zero, which results
 214 in the dynamics becoming undefined at the optima.

215 To enforce these conditions, we make the following design decisions regarding V :

216 **No local optima.** We represent V via an input-convex neural network (ICNN)
 217 function $g : \mathbb{R}^n \rightarrow \mathbb{R}$ [1], which enforces the condition that $g(x)$ be convex in its
 218 inputs x . Such a network is given by the recurrence

$$\begin{aligned}
 z_1 &= \sigma_0(W_0x + b_0) \\
 z_{i+1} &= \sigma_i(U_i z_i + W_i x + b_i), i = 1, \dots, k-1. \\
 g(x) &\equiv z_k
 \end{aligned}
 \tag{1.11}$$

220 For layer $i+1$: W_i are weights mapping from the input x to the $i+1$ layer activations;
 221 U_i are positive weights mapping previously layer activations z_i to the next layer; b_i
 222 are real-valued biases; and σ_i are convex, monotonically non-decreasing non-linear
 223 activations such as the ReLU or smooth variants. It is straightforward to show that
 224 with this formulation, g is convex in x [1], and indeed any convex function can be
 225 approximated by such networks [5].

226 **Positive definite.** The ICNN property enforces that V has only a single global
 227 optimum; for V to be positive definite, we must also enforce that this optimum is
 228 at $x = 0$. We could fix this by removing the bias term from Equation 1.11, but
 229 this would mean we could no longer represent arbitrary convex functions. We could
 230 also shift whatever global minimum to the origin, but that would require finding
 231 finding the global minimum during training, which itself is computationally expensive.
 232 Instead, we take an alternative approach: we shift the function such that $V(0) = 0$,
 233 and add a small quadratic regularization term to ensure strict positive definiteness.

$$V(x) = \sigma_{k+1}(g(x) - g(0)) + \epsilon \|x\|_2^2.
 \tag{1.12}$$

235 where σ_k is a positive convex non-decreasing function with $\sigma_k(0) = 0$, g is the ICNN
 236 defined previously, and ϵ is a small constant. These terms together still enforce
 237 (strong) convexity and positive definiteness of V .

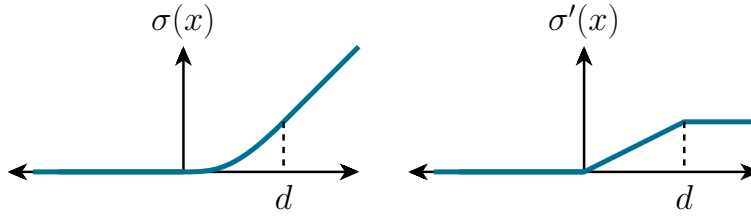


Figure 1.2: Rectified Huber Unit (ReHU), necessary for continuously differentiable Lyapunov functions.

238 **Continuously differentiable.** Although not always required, several of the condi-
 239 tions for Lyapunov stability are simplified if V is continuously differentiable. ReLU
 240 is discontinuous around 0, and the soft-plus smoothed ReLU is not zero at the origin.
 241 We use a smoothed version with quadratic knee in $[0, d]$, called the Rectified Huber
 242 Unit (ReHU):

$$243 \quad \sigma(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x^2/2d & \text{if } 0 < x < d. \\ x - d/2 & \text{otherwise} \end{cases} \quad (1.13)$$

244 An illustration of this activation is shown in Figure 1.2.

245 **[Optional] Warped input space.** Our construction so far guarantees that the
 246 Lyapunov function has no local optima by making it convex. This is sufficient but not
 247 necessary, and it may even impose too strict a constraint on the learned dynamics.
 248 We can relax this function by allowing the input to the ICNN to be warped by any
 249 continuously differentiable invertible function $F : \mathbb{R}^n \times \mathbb{R}^n$. i.e., using

$$250 \quad V(x) = \sigma_{k+1}(g(F(x)) - g(F(0))) + \epsilon \|x\|_2^2. \quad (1.14)$$

251 as the Lyapunov function. Invertibility ensures that the level sets of V , which are
 252 convex, map to contiguous regions of the composite function $g \circ F$. This allows the
 253 resultant Lyapunov function to be non-convex without having any optima other than
 254 the global.

255 With these conditions in place, we have the following result.

256 **Theorem 1.** *The dynamics defined by*

$$257 \quad \dot{x} = f(x) \quad (1.15)$$

258 *are globally exponentially stable to the equilibrium point $x = 0$. Where f is from*
 259 *Eqn. equation 1.10 and V is from Eqn. equation 1.12 or Eqn. equation 1.14, and \hat{f}*
 260 *and V functions have finite, bounded weights.*

261 *Details.* The proof is straightforward, and relies on the properties of the networks
 262 created above. First, note that by our definitions we have, for some M ,

$$263 \quad \epsilon \|x\|_2^2 \leq V(x) \leq M \|x\|_2^2 \quad (1.16)$$

264 where the lower bound follows from Eqn. 1.12 and the fact that g is positive. The
 265 upper bound follows from the fact that the ReHU activation is linear for large x and
 266 quadratic around 0. This fact in turn implies that $V(x)$ behaves linearly as $\|x\| \rightarrow \infty$,
 267 and is quadratic around the origin, so can be upper bounded by some quadratic
 268 $M \|x\|_2^2$.

269 The fact the V is continuously differentiable means that $\nabla V(x)$ (in f) is defined
 270 everywhere, bounds on $\|\nabla V(x)\|_2^2$ for all x follows from the the Lipschitz property of
 271 V , the fact that $0 \leq \sigma'(x) \leq 1$, and the $\epsilon \|x\|_2^2$ term

$$272 \quad \epsilon \|x\|_2 \leq \|\nabla V(x)\|_2 \leq \sum_{i=1}^k \prod_{j=i}^k \|U_j\|_2 \|W_i\|_2 \quad (1.17)$$

273 where $\|\cdot\|_2$ denotes the operator norm when applied to a matrix. This implies that
 274 the dynamics are defined and bounded everywhere owing to the choice of function \hat{f} .

275 Now, consider some initial state $x(0)$. The definition of f implies that

$$276 \quad \frac{d}{dt} V(x(t)) = \nabla V(x)^T \frac{d}{dt} x(t) = \nabla V(x)^T f(x) \leq -\alpha V(x(t)). \quad (1.18)$$

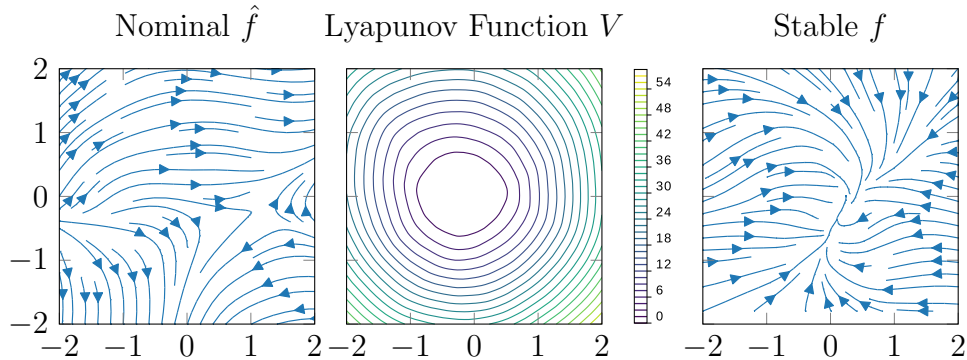


Figure 1.3: (left) Nominal dynamics \hat{f} for random network; (center) Convex positive definite Lyapunov function generated by random ICNN with constraints from Section 1.3.1; (right) Resulting stable dynamics f .

277 Integrating this equation gives the bound

$$278 \quad V(x(t)) \leq V(x(0))e^{-\alpha t} \quad (1.19)$$

279 and applying the lower and upper bounds gives

$$280 \quad \epsilon \|x(t)\|_2^2 \leq M \|x(0)\|_2^2 e^{-\alpha t} \implies \|x(t)\|_2 \leq \frac{M}{\epsilon} \|x(0)\|_2 e^{-\alpha t/2} \quad (1.20)$$

281 as required for global exponential convergence. \square

282 1.4 Empirical results

283 We illustrate our technique on several example problems, first highlighting the
 284 (inherent) stability of the method for random networks, demonstrating learning on
 285 simple n -link pendulum dynamics, and finally learning high-dimensional stable latent
 286 space dynamics for dynamic video textures via a VAE model.

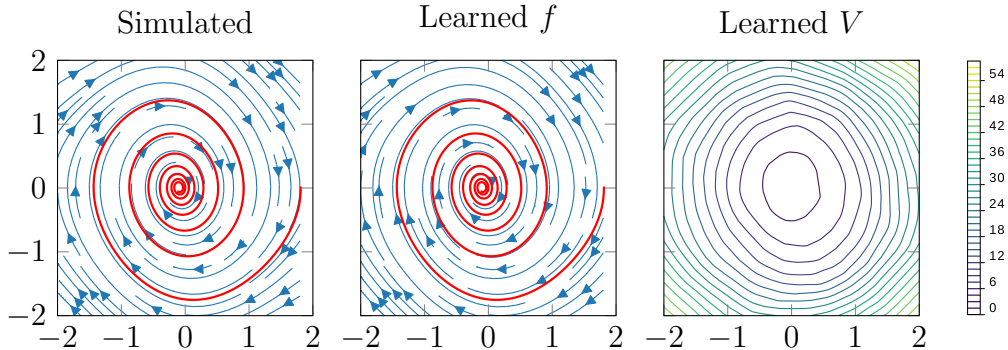


Figure 1.4: Dynamics of a simple damped pendulum. From left to right: the dynamics as simulated from first principles, the dynamics model f learned by our method, and the Lyapunov function V learned by our method (under which f is non-expansive).

287 1.4.1 Random networks

288 Although we mention this only briefly, it is interesting to visualize the dynamics
 289 created by random networks according to our process, i.e., before any training at all.
 290 Because the dynamics models are inherently stable, these random networks lead to
 291 stable dynamics with interesting behaviors, illustrated in Figure 1.3. Specifically, we
 292 let \hat{f} be defined by a fully connected network and V be an ICNN. Both networks have
 293 two hidden layers with 100 nodes each, and are initialized by the Kaiming uniform
 294 initialization [18]). The U weights in the ICNN are further subject to a softplus unit
 295 to make them positive.

296 1.4.2 n -link pendulum

297 Next we look at the ability of our approach to model a physically-based dynamical
 298 system, specifically the n -link pendulum. A damped, rigid n -link pendulum's state
 299 x can be described by the angular position θ_i and angular velocity $\dot{\theta}_i$ of each link i .
 300 As before \hat{f} and the Lyapunov function V have two hidden layers of 100 nodes, with
 301 properties described in Section 1.3.1. Models are trained with pairs of data (x, \dot{x})
 302 produced by the symbolic algebra solver `sympy`, using simulation code adapted from
 303 [55].

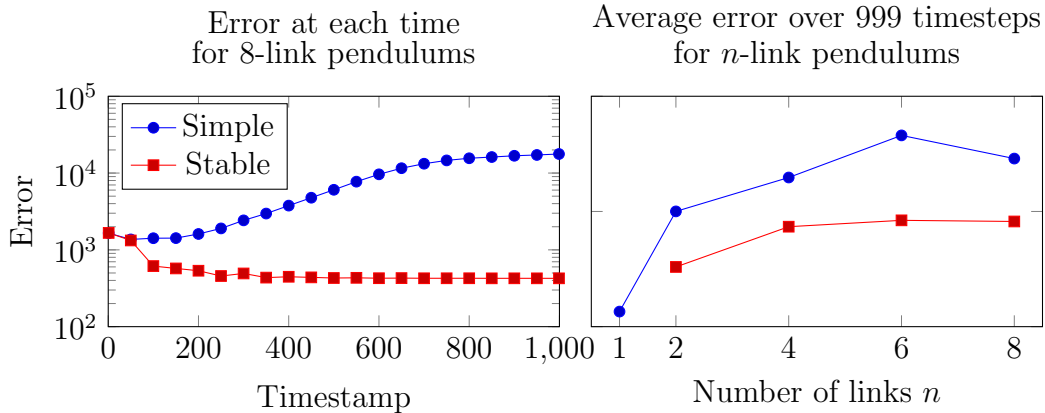


Figure 1.5: Error in predicting $\theta, \dot{\theta}$ in 8-link pendulum at each timestep (left); and average error over 999 timesteps as the number of links in the pendulum increases (right).

304 In Figure 1.4, we compare the simulated dynamics with the learned dynamics in the
 305 case of a simple damped pendulum (i.e. with $n = 1$), showing both the vector field
 306 and a single simulated trajectory, and draw a contour plot of the learned Lyapunov
 307 function. As seen, the system is able to learn dynamics that can accurately predict
 308 motion of the system even over long time periods.

309 We also evaluate the learned dynamics quantitatively varying n and the time horizon
 310 of simulation. Figure 1.5 presents the total error over time for the 8-link pendulum,
 311 and the average cumulative error over 1000 time steps for different values of n . While
 312 both the simple and our stable models show increasing mean error at the start of
 313 the trajectory, our model is able to capture the contraction in the physical system
 314 (implied by conservation of energy) and in fact exhibits decreasing error towards
 315 the end of the simulation (the true and simulated dynamics are both stable). In
 316 comparison, the error in the simple model increases.

317 1.4.3 Video Texture Generation

318 Finally, We apply our technique to stable video texture generation, using a Variational
 319 Auto-Encoder (VAE) [23] to learn an encoding for images, and our stable network to

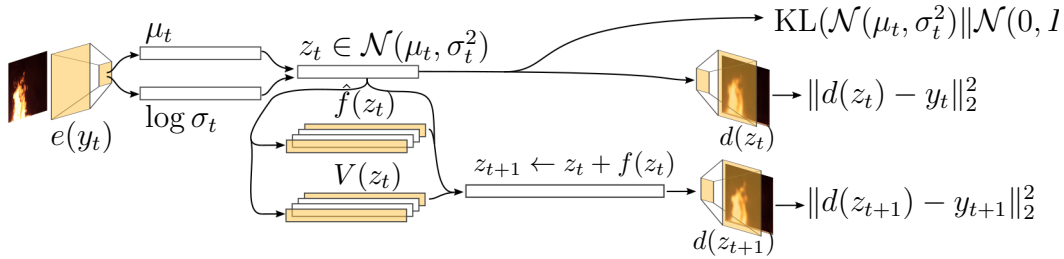


Figure 1.6: Structure of our video texture generation network. The encoder e and decoder d form a Variational Autoencoder, and the stable dynamics model f is trained together with the decoder to predict the next frame in the video texture.

320 learn a dynamics model in encoding-space. Given a sequence of frames (y_0, y_1, \dots) ,
 321 we feed the network the frame at time t and train it to reconstruct the frames at
 322 time t and $t + 1$. Specifically, we consider a VAE defined by the encoder $e : \mathcal{Y} \rightarrow \mathbb{R}^{2n}$
 323 giving mean and variance $\mu, \log \sigma_t^2 = e(y_t)$, latent state $z_t \in \mathbb{R}^n \sim \mathcal{N}(\mu_t, \sigma_t^2)$, and
 324 decoder $d : \mathbb{R}^n \rightarrow \mathcal{Y}$, $y_t \approx d(z_t)$. We train the network to minimize both the standard
 325 VAE loss (reconstruction error plus a KL divergence term), but *also* minimize the
 326 reconstruction loss of a next predicted state. We model the evolution of the latent
 327 dynamics at $z_{t+1} \approx f(z_t)$, or more precisely $y_{t+1} \approx d(f(z_t))$. In other words, as
 328 illustrated in Figure 1.6, we train the full system to minimize

$$\begin{aligned}
 329 \quad & \underset{e, d, \hat{f}, V}{\text{minimize}} \sum_{t=1}^{T-1} \left(\text{KL}(\mathcal{N}(\mu_t, \sigma_t^2 I) \| \mathcal{N}(0, I)) + \mathbf{E}_z [\|d(z_t) - y_t\|_2^2 + \|d(f(z_t)) - y_{t+1}\|_2^2] \right) \\
 & \hspace{20em} (1.21)
 \end{aligned}$$

330 We train the model on pairs of successive frames sampled from videos. To generate
 331 video textures, we seed the dynamics model with the encoding of a single frame and
 332 numerically integrate the dynamics model to obtain a trajectory. The VAE decoder
 333 converts each step of the trajectory into a frame. In Figure 1.7, we present sample
 334 stable trajectories and frames produced by our network. For comparison, we also
 335 include an example trajectory and resulting frames when the dynamics are modelled
 336 without the stability constraint (i.e. letting f in the above loss be a generic neural

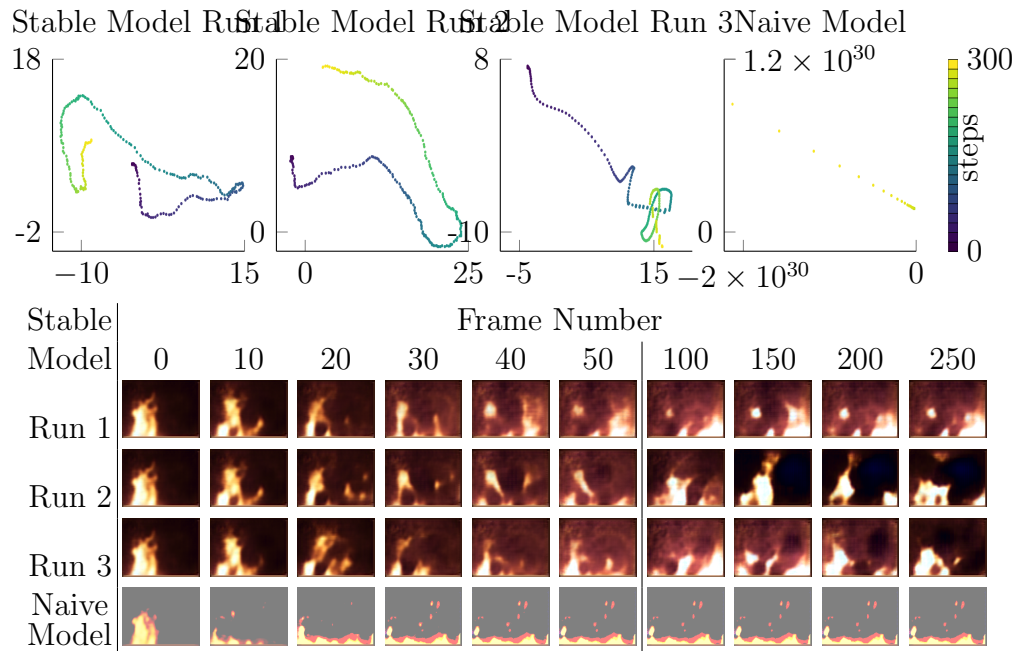


Figure 1.7: Samples generated by our stable video texture networks, with associated trajectories above. The true latent space is 320-dimensional; we project the trajectories onto a two-dimensional plane for display. For comparison, we present the video texture generated using an unconstrained neural network in place of our stable dynamics model.

337 network). For the naive model, the dynamics quickly diverge and produce a static
338 image, whereas for our approach, we are able to generate different (stable) trajectories
339 that keep generating realistic images over long time horizons.

340 1.5 Conclusion

341 We proposed a method for learning stable non-linear dynamical systems defined by
342 neural network architectures. The approach jointly learns a convex positive definite
343 Lyapunov function along with dynamics constrained to be stable according to these
344 dynamics everywhere in the state space. We show that these models can be integrated
345 into other deep architectures such as VAEs, and learn complex latent space dynamics
346 is a fully end-to-end manner. Although we have focused here on the autonomous
347 (uncontrolled) setting, the method opens several directions for future work, such as
348 integration into dynamical systems for control or reinforcement learning settings.
349 Have stable systems as a “primitive” can be useful in a large number of contexts, and
350 combining these stable systems with the representational power of deep networks
351 offers a powerful tool in modeling and controlling dynamical systems.

352 1.6 Adaptation to Stable Control and RL

353 After the successes of our stable dynamics model, we attempted to extend it to also
354 learn stable policies and value functions. The intuitive extension to this is to replace
355 the dynamics model \hat{f} with fixed (known) dynamics \tilde{f} and a learnable policy network
356 π . That is, we train to minimize:

$$357 \quad \text{ReLU}(\nabla V(x)^T \tilde{f}(x, \pi) + \alpha V(x)) \quad (1.22)$$

358 given traces from simulated dynamics. We also transformed the dynamics so that
359 the goal state was positioned at the origin, choosing suitable transformations for the
360 dynamics and Lyapunov functions. As required by the approach, we attempted to
361 train it from trajectory samples to minimize the error over one step.

362 We were able to successfully learn stabilizing controllers for toy examples such as a
363 simple damped pendulum and for the cartpole problem. Unfortunately, we were not
364 able to learn a swing-up controller for either environment, or any type of controller
365 for an Acrobot¹ or more complex locomotion tasks. We observed that the training
366 would consistently fail in the same way: the nominal dynamics function would diverge
367 to the point of uselessness, followed by the learned Lyapunov function collapsing to a
368 trivial function.

369 This persisted despite any amount of regularization, hyperparameter tuning, and
370 even across a variety of environments. Contemporary efforts in the literature were
371 similarly unable to scale this approach to locomotion tasks. The consistent failure
372 of this method suggested that an underlying principle was being violated, and that
373 regularization was not able to address that. We eventually investigated how the
374 difference in distributions between the data used to train the purportedly stable
375 controller and the policy the controller was attempting to learn, which led us to the
376 work in the next chapter.

¹A two-link pendulum with a single actuator in the middle joint.

377 Chapter 2

378 The Pitfalls of Regularization in 379 Off-Policy Temporal Difference 380 Learning

381 Temporal Difference (TD) learning is ubiquitous in reinforcement learning, where it is
382 often combined with off-policy sampling and function approximation. Unfortunately
383 learning with this combination (known as the *deadly triad*), exhibits instability and
384 unbounded error. To account for this, modern RL methods often implicitly (or
385 sometimes explicitly) assume that regularization is sufficient to mitigate the problem
386 in practice; indeed, the standard deadly triad examples from the literature can
387 be “fixed” via proper regularization. In this paper, we introduce a series of new
388 counterexamples to show that the instability and unbounded error of TD methods
389 is *not* solved by regularization. We demonstrate that, in the off-policy setting with
390 linear function approximation, TD methods can fail to learn a non-trivial value
391 function under *any* amount of regularization; we further show that regularization
392 can induce divergence under common conditions; and we show that one of the most
393 promising methods to mitigate this divergence (Emphatic TD algorithms) may also
394 diverge under regularization. We further demonstrate such divergence when using

395 neural networks as function approximators. Thus, we argue that regularization in TD
396 methods needs to be reconsidered, given that it is insufficient to prevent divergence
397 and may itself introduce instability. There needs to be much more care in the
398 application of regularization to RL methods.

399 *From “The Pitfalls of Regularization in Off-Policy TD Learning” by Manek and*
400 *Kolter (2022)*

401 2.1 Introduction

402 Temporal Difference (TD) learning is a method for learning expected future-discounted
403 quantities from Markov processes, using transition samples to iteratively improve
404 estimates. This is most commonly used to estimate expected future-discounted
405 rewards (the *value function*) in Reinforcement Learning (RL). Advances in RL allow
406 us to use powerful function approximators, and also to use sampling strategies other
407 than naively following the Markov process (MP). When TD, function approximation,
408 and off-policy training are all combined, learned functions exhibit severe instability
409 and divergence, as classically observed by Williams and Baird III [58] and Tsitsiklis
410 and Van Roy [53]. This combination is known in the literature as the *deadly triad* [48,
411 pg. 264], and while many contemporary variants of TD are designed to converge
412 despite the instability, the quality of the solution at convergence may be arbitrarily
413 poor.

414 A common technique to avoid unbounded error is ℓ_2 *regularization* [52], i.e. penalizing
415 the squared norm of the weights in addition to the TD error. This is generally
416 understood to bound the worst-case error in exchange for biasing the model and
417 potentially increasing the error everywhere else. When used on three common
418 examples of the deadly triad [24, 58, 48, pg.260], regularization appears to mitigate
419 the worst aspects of the divergence in practice. Consequently, it has become an
420 essential assumption made by many RL algorithms [8, 33, 50, 60, 63, 62, 27] and is
421 seen as routine and innocuous.

422 We argue that this perspective on regularization in off-policy TD is fundamentally
423 mistaken. While regularization is indeed reasonably well-behaved and innocuous in
424 classic fully-supervised contexts, the use of bootstrapping in TD means that even
425 small amounts of model bias induced by regularization can cause divergence. This
426 is an oft-ignored phenomenon in the literature, and so we introduce a series of new
427 counterexamples (summarized in Table 2.1) to show how regularization can have coun-
428 terintuitive and destructive effects in TD. We show that vacuous solutions and training
429 instability are *not* solved by the use of regularization; that applying regularization can

430 sometimes induce divergence and increase worst-case error; and that Emphatic TD
431 algorithms—which are the most promising solution to this divergence—can themselves
432 diverge when regularized. We finally also illustrate misbehaving regularization in the
433 context of neural network value function approximation, demonstrating the general
434 pitfalls of regularization possible in RL algorithms. Regularization needs to be treated
435 cautiously in the context of RL, as it behaves differently than in supervised settings.

436 Our counterexamples demonstrate these core ideas:

437 **TD learning off-policy can be unstable and/or have unbounded error even**
438 **when it converges.** Following well-established methods we show there is some
439 off-policy distribution under which TD with linear value function approximation
440 diverges *and* learns a model with unbounded error (even if it were able to converge
441 to the TD fixed point). This concisely demonstrates key features of the training
442 error: the error is small when the distribution is close to on-policy, but the error
443 diverges around specific off-policy distributions. The intuition behind this, explained
444 in Section 2.3, is that the off-policy¹ TD update involves a projection operation that
445 depends on the sampling distribution and can be arbitrarily far away from the true
446 value. This basic fact has already been established by past work [58, 24], but our
447 example is based upon a particular simple three-state MP, drawn in Figure 2.1a.

448 **Regularization cannot always mitigate off-policy training error.** We next
449 introduce regularization into our setting, and show how it changes the relationship
450 between training error and off-policy training. As explained in Section 2.2, we penalize
451 the ℓ_2 -norm of learned (linear) weights with some coefficient η ; as η increases, the
452 learned weights approach zero. However, in **Example 1**, we show that there exists
453 an off-policy distribution such that for any $\eta \geq 0 < \infty$, the regularized TD fixed
454 point attains strictly higher approximation error than the zero solution (i.e., the
455 infinitely regularized point). We call such examples *vacuous*. In other words, *vacuous*
456 *value functions never do better than guessing zero for all states, for any amount of*

¹We consider a sampling distribution to be *on-policy* if it follows the stationary distribution of the MP; we do not explicitly consider a separate policy in this paper.

457 *regularization.*

458 We further analyze this vacuous example in the context of the algorithm in [62]. In
459 this work, the authors assume the use of regularization to derive bounds on the learned
460 error under off-policy sampling. Although these bounds are technically correct in the
461 case of our counterexample, they are very loose, at about 2000 times the threshold of
462 vacuity. This highlights the challenge of formally relying on regularization to bound
463 model error.

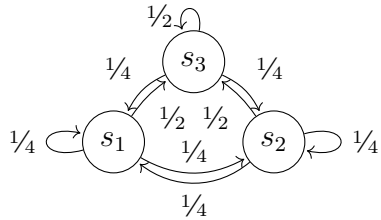
464 **Small amounts of regularization can cause model divergence or large errors.**

465 There is a general implicit assumption in much ML literature that regularization
466 monotonically shrinks learned weights. This intuition comes from classic fully-
467 supervised machine learning where it typically holds. But because TD bootstraps
468 value estimates (i.e. learns values using its own output), it is possible for small
469 amounts of bias to be arbitrarily magnified. We dub this phenomenon “small-eta
470 error” and illustrate it in **Example 2**. We relate this to the presence of negative
471 eigenvalues in an intermediate step of the solution and show that, in some settings, the
472 error of the TD solution may be relatively small when applied with no regularization
473 but adding regularization causes the model to have worse error than the zero solution.

474 One common solution to this problem is to lower-bound η to guarantee that regular-
475 ization behaves monotonically. However, we further show that such a lower bound
476 may occur after the point of vacuity: a model that is not vacuous becomes vacuous
477 for any regularization parameter above this lower bound. We also show that it is not
478 always possible to select a single η *a priori*, with examples of mutually-incompatible
479 off-policy distributions where there is no η that achieves better than vacuous or
480 nearly-vacuous results at different distributions.

481 **Emphatic-TD-based algorithms are vulnerable to instability from reg-
482 ularization.**

Emphatic-TD [49] fundamentally solves the problem of training
483 off-policy by resampling TD updates so they appear to be on-policy. This technique
484 requires an emphasis model that decides how to scale each TD update, and learning



(a) Three-state MP.

$$\frac{1}{4} \begin{bmatrix} 1 & 1 & 2 \\ 1 & 1 & 2 \\ 1 & 1 & 2 \end{bmatrix} \quad (2.1)$$

(b) Three-state MP.

Figure 2.1: Our three-state counterexample Markov Process. We use this to illustrate how TD models can fail despite common mitigating strategies with linear function approximation.

485 this has been the key challenge preventing widespread adoption of Emphatic-TD. A
 486 recent paper [63] proposed learning this emphasis model using “reversed” TD while
 487 simultaneously learning the value model using regular TD. The resultant algorithm
 488 is called COF-PAC, and employs regularization to ensure that the two TD models
 489 eventually converge.

490 We show that regularization, while necessary, can be harmful for such models in
 491 **Example 3**. Specifically, we construct a model that converges to the correct solution
 492 without regularization but to an arbitrarily poor solution when regularized. The
 493 intuition behind this is that regularizing the emphasis model changes the effective
 494 distribution of the TD updates to the value model, which can cause the value model
 495 to have arbitrarily large error. We complete the example by showing that regularizing
 496 the value function separately does not restore performance.

497 **Regularization can cause model divergence in neural networks.** So far
 498 most analysis of the deadly triad in the literature focuses on the linear case. We
 499 extend our example to a nine-state Markov chain (shown in Figure 2.8), and show how
 500 the previously identified problems persist into the neural network case in **Example 4**.
 501 We show two key similarities: first, models trained at certain off-policy distributions
 502 may be vacuous. Second, small amounts of regularization counterintuitively *increase*
 503 error. This illustrates Example 2 in the NN case.

-
-
- Example 1** There exist off-policy distributions under which TD learns a *vacuous* model (one which—despite any amount of regularization—never does better than guessing zeros).
- Example 2** Small values of the regularization parameter η can make TD diverge in models that otherwise converge. This is an unavoidable effect of bootstrapping in TD, and setting a lower-bound to exclude this may render models vacuous.
- Example 3** Emphatic-TD-inspired algorithms are a promising way to reweigh samples and mitigate the effects of training off-policy. But if this reweighing is learned using TD, then using regularization can bias the emphasis model and cause the value model itself to diverge.
- Example 4** Training instability and increased error due to the deadly triad also occur when neural networks are used. We construct an empirical example and draw qualitative comparisons.
-
-

Table 2.1: Summary of theorems.

504 2.2 Preliminaries and Notation

505 Consider the n -state Markov chain $(\mathcal{S}, P, R, \gamma)$, with state space \mathcal{S} , state-dependent
 506 reward $R : \mathcal{S} \rightarrow \mathbb{R}$, and discount factor $\gamma \in [0, 1]$. $P \in \mathbb{R}^{n \times n}$ is the transition matrix,
 507 with P_{ij} encoding the probability of moving from state i to j . We wish to estimate
 508 the value function $V : \mathcal{S} \rightarrow \mathbb{R}$, defined as the expected discounted future reward of
 509 being in each state: $V(s) \doteq \mathbf{E} [\sum_{t=0}^{\infty} \gamma^t R(s_t) | s_0 = s]$. A key property is that it follows
 510 the Bellman equation:

$$511 \quad V = R + \gamma PV \quad (2.2)$$

Using linear function approximation to learn V , we assume a matrix of feature-vectors $\Phi \in \mathbb{R}^{n \times k}$ that is fixed, and a vector of parameters $w \in \mathbb{R}^k$ that is learned. The Bellman equation is then:

$$\Phi w = R + \gamma P \Phi w \tag{2.3}$$

When w is learned with TD, this equation is only valid if the TD updates are *on-policy* (that is, they are distributed according to the steady-state probability of visiting each state, written as $\pi \in \mathbb{R}^n$). In the general case, where TD updates follow a (possibly) different distribution $\mu \in \mathbb{R}_0^n$, the TD solution is a fixed point of the Bellman operator followed by a projection [24]:

$$\Phi w = \Pi_\mu (R + \gamma P \Phi w) \tag{2.4}$$

where the matrix $\Pi_\mu = \Phi(\Phi^\top D \Phi)^{-1} \Phi^\top D$ projects the Bellman backup onto the column-space of Φ , reweighed by the diagonal matrix $D = \text{diag}(\mu)$. This yields the closed-form solution:

$$w = A^{-1} \vec{b} \tag{2.5}$$

Where $A = \Phi^\top D(I - \gamma P)\Phi$ and $\vec{b} = \Phi^\top D R$. When this solution is subject to ℓ_2 regularization, some non-negative η is added to ensure the matrix being inverted is positive definite:

$$w^*(\eta) = (A + \eta I)^{-1} \vec{b} \tag{2.6}$$

As will be important later, we note that as η increases it drives $w^*(\eta)$ towards zero.

2.3 Our Counterexamples

Under deadly triad conditions are present, TD may learn a value function with arbitrarily large error even if the true value function can be represented with low

526 error. Consider the three-state MP in Figure 2.1a, which we instantiate with the
 527 value function $V = [1, 2.2, 1.05]^\top$ and discount factor $\gamma = 0.99$. The reward function
 528 is computed as $R \leftarrow (I - \gamma P)V$. We choose a basis Φ with small representation error
 529 $\|\Pi_\mu V - V\| \leq \epsilon$:

$$530 \quad \Phi = \begin{bmatrix} 1 & 0 \\ 0 & -2.2 \\ 1/2(1.05 + \epsilon) & -1/2(1.05 + \epsilon) \end{bmatrix} \quad \text{where } \epsilon > 0 \quad (2.7)$$

531 We first consider the unregularized ($\eta = 0$) case, closely following the derivation
 532 in [24]. We wish to show there is some sampling distribution μ such that error in the
 533 learned value function is unbounded. To do this, we set $\mu = [0.56(1 - p), 0.56p, 0.44]$,
 534 where $p \in (0, 1)$. We set $\epsilon = 10^{-4}$ and find p around which A is ill-conditioned by
 535 solving $\det(A) = 0$:

$$536 \quad p = 0.102631 \quad \vee \quad p = 0.807255 \quad (2.8)$$

537 A^{-1} (and consequently the error) can be made arbitrarily large by selecting p close to
 538 these values, which completes the introductory example. Now we look at the behavior
 539 of TD under regularization, which is the main contribution of this chapter.

540 **2.3.1 Regularization cannot always mitigate off-policy train-** 541 **ing error.**

542 There is a belief in the literature that regularization is a trade-off between reducing
 543 the blow-up of asymptotic errors and accurately learning the value function every-
 544 where else [8, 62]. However, this belief does not accurately capture the nature of
 545 regularization: we show that it is possible to learn models that never perform better
 546 than always guessing zero despite any amount of regularization. That is, the TD
 547 error at all η is at least as much as the error as $\eta \rightarrow \infty$. We call such models *vacuous*.

548 **Example 1.** We use the same setting as in Section 2.3. When TD is regularized,

549 there may exist some off-policy distribution at which TD learns a vacuous model. In
 550 notation:

$$551 \quad \|\Phi w^*(\eta) - V\| \geq \lim_{\eta \rightarrow \infty} \|\Phi w^*(\eta) - V\| = \|\Phi \vec{0} - V\| = \|V\| \quad \forall \eta \in \mathbb{R}_0^+ \quad (2.9)$$

552 *Details.* We use the same setting as in Section 2.3. We observe that $\hat{w} = [1, -1]^\top$
 553 minimizes the least-squares error $\|\Phi \hat{w} - V\|$, and further observe that a sufficient (but
 554 not necessary) condition for a solution to be vacuous is that $\hat{w}^\top w^*(\eta) \leq 0$. Solving:

$$555 \quad 0 = \hat{w}^\top w^*(\eta) = \frac{\eta p - 0.233\eta - 0.304p^2 + 0.276p - 0.025}{\eta^2 + 1.44\eta p + 0.215\eta - 0.193p^2 + 0.175p - 0.016} \quad (2.10)$$

$$556 \quad \implies p \in \{0.102636, \dots\} \quad (2.11)$$

557 We verify that TD is vacuous at $p = 0.102636$ by computing the TD error at
 558 convergence:

$$559 \quad \|\Phi w^*(\eta) - V\|^2|_{p=\bar{p}} = \frac{\eta^2(0.148 + 0.744\eta + \eta^2)}{\eta^2(0.132 + 0.727\eta + \eta^2)} \|V\|^2 \geq \|V\|^2 \quad (\forall \eta \in \mathbb{R}^+) \quad (2.12)$$

560 Since the fraction term in Equation 2.12 is obviously improper, we can conclude
 561 that our example will always have at least $\|V\|$ error over all η , and is therefore
 562 vacuous. \square

563 We note that the error is not defined at $\eta = 0$ because this corresponds to a model
 564 divergence similar to our introductory example. In practice, the TD fixed point will
 565 still converge to a vacuous solution:

$$566 \quad \lim_{\eta \rightarrow 0} \|\Phi w^*(\eta) - V\|^2 = \frac{0.148}{0.132} \|V\|^2 > \|V\|^2 \quad (2.13)$$

567 **Geometry of vacuous linear models.**

568 We begin by noting that we can easily find the solution \hat{w} that minimizes the least-
 569 squares error $\|\Phi \hat{w} - V\|$. If we consider this solution as a vector (as drawn in

570 Figure 2.2a), we can immediately see that there is an ℓ_2 -ball around \hat{w} corresponding
571 to the set of $w^*(\eta)$ with no more than $\|V\|$ error.

572 Similarly, we can trace the trajectory that the TD solution $w^*(\eta)$ takes as η is
573 increased from 0 to ∞ . We know that, as $\eta \rightarrow \infty$, $w^*(\eta)$ is crushed to zero and so
574 all trajectories must eventually terminate at the origin. When regularized models
575 are not vacuous, the trajectory intersects the non-vacuous-error ball. We see this in
576 trajectory 2, where the error briefly dips below $\|V\|$ in Figure 2.2b.

577 Intuitively, a sufficient condition for a solution to be vacuous is that it remains in the
578 half-space that is tangent to and excludes the non-vacuous parameter ball. This is
579 equivalent to finding some distribution μ such that $\hat{w}^\top w^*(\eta) \leq 0$ for all η , which we
580 numerically solve to obtain the model in trajectory 1. From Figure 2.2a we can see
581 the trajectory remains in the half-space, and from Figure 2.2b we can see that the
582 error is never less than $\|V\|$. Trajectory 1 is a vacuous example.

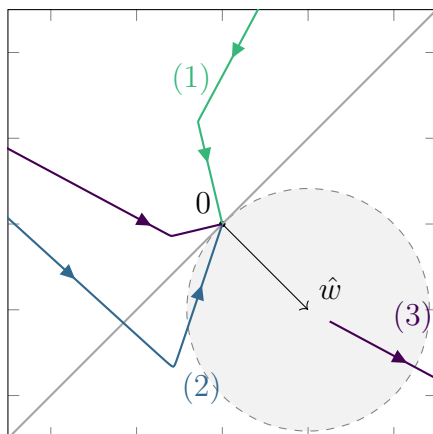
583 We observe that Example 1, because it remains entirely in the half-space $\hat{w}^\top w^*(\eta) \leq 0$,
584 could easily be generalized to other forms of regularization. We leave this for future
585 work.

586 This intuition does not persist in the neural network case (discussed in Section 2.3.4).
587 In that case, the relationship between parameters and error does not admit a clean
588 non-vacuous ball, but instead a deeply non-linear set of states. The resultant geometry
589 does not admit a clean, intuitive, explanation.

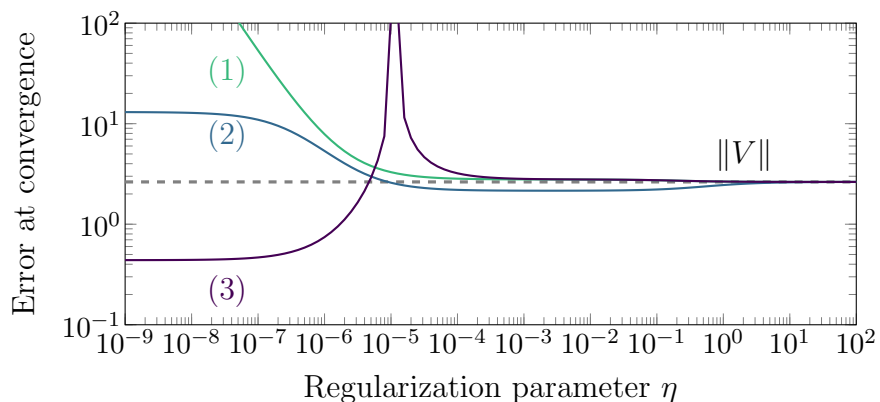
590 **A second example.**

591 We present a second example where the error is stationary with respect to the
592 regularization parameter. This is worse than Example 1 because we are able to show
593 that the point the model converges to is *independent* of regularization. This example
594 is the natural extension of that of Kolter [24].

595 *Details.* We use the same setting as in Section 2.3, except the value function is $V =$



(a) As η increases, $w^*(\eta)$ traces different trajectories at different μ . \hat{w} minimizes the error, and we shade the area with TD error less than $\|V\|$.



(b) We plot the error curves corresponding to the three $w^*(\eta)$ trajectories, along with $\|V\|$. Trajectory 1 is vacuous because the error is at least $\|V\|$ for all η .

Figure 2.2: Plotting the trajectory of the parameters on above and the errors below, we show how our counterexample 1 is never better than $\|V\|$ because it remains in half-space where $\hat{w}^\top w^*(\eta) \leq 0$. For comparison, we show trajectory 2 that is improved by regularization, and 3, which exhibits small- η errors. (The trajectories are distorted, so the errors in the two plots are not directly comparable.)

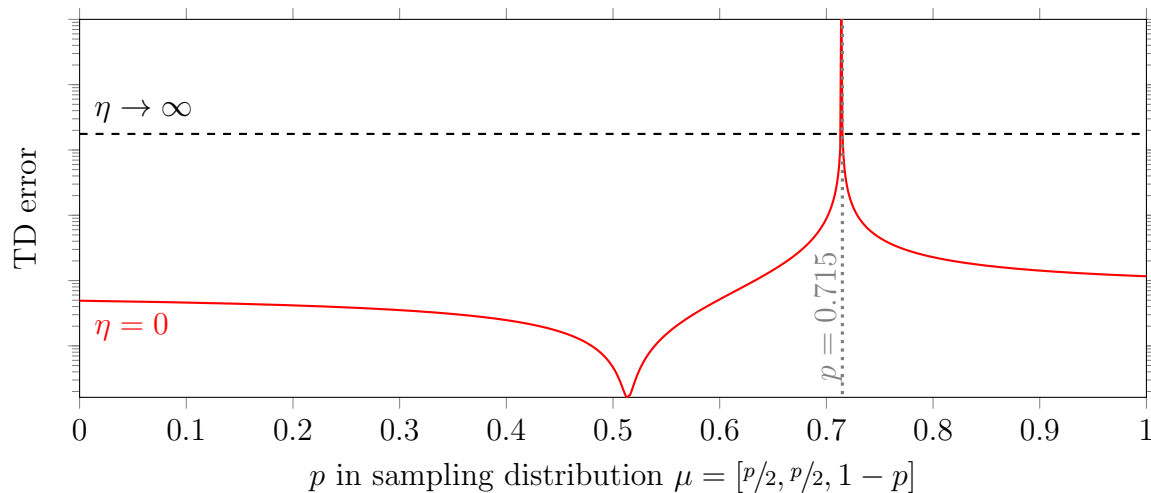


Figure 2.3: We plot TD error against p for our three-state MP with $\epsilon = 10^{-4}$. This shape is similar to that in [24]. There is a minima close to π ($p \approx 0.5$), and an asymptote at the singularity ($p \approx 0.715$). At different levels of regularization the error function moves between the unregularized case ($\eta = 0$) and the limiting case ($\eta \rightarrow \infty$), as analyzed in Section 2.3.1. We show that there is some p at which the error is never below the $\eta \rightarrow \infty$ line.

596 $[1, 1, 1.05]^\top$ and basis Φ selected to have small representation error $\|\Pi_D V - V\| \leq \epsilon$:

$$597 \quad \Phi = \begin{bmatrix} 1 & 0 \\ 0 & -1 \\ 1/2(1.05 + \epsilon) & -1/2(1.05 + \epsilon) \end{bmatrix} \quad \text{where } \epsilon > 0 \quad (2.14)$$

598 . We set $\epsilon = 10^{-4}$ and write down $w^*(\eta)$ in terms of g , a scalar function of η and p :

$$599 \quad w^*(\eta) = (A + \eta I)^{-1} \vec{b} = \frac{(2\eta + p)(0.925 - 1.29p)}{100\eta^2 + 47.4p\eta + 1.85\eta - 1.30p^2 + 0.927p} \cdot \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (2.15)$$

$$600 \quad \equiv g(p, \eta) \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (2.16)$$

601 When $g(p, \eta) \leq 0$, the TD solution is vacuous. We show that directly:

$$602 \quad \|\Phi w^*(\eta) - V\| = \|g(p, \eta) \Phi * [1, -1]^\top - \Phi * [1, -1]^\top\| = \|g(\eta) - 1\| \cdot \|V\| \quad (2.17)$$

603 When $g(p, \eta) \leq 0$, then $\|g(p, \eta) - 1\| \geq 1$ for all η and the TD solution is vacuous.
 604 We find such a solution by noting the numerator has two roots in p , one of which
 605 corresponds to a vacuous solution: $g(0.715083, \eta) = 0$ ($\forall \eta$), and this completes the
 606 example!

607 In this setting, when TD updates follow the sampling distribution $p \approx 0.715083$, the
 608 error of the model at convergence is always $\|V\|$ regardless of regularization. Our
 609 example converges to the same vacuous value regardless η . \square

610 We present this graphically in Figure 2.3, where we plot the relationship between the
 611 off-policy distribution and the error at the TD fixed point. We plot the error with no
 612 regularization ($\eta = 0$) and the limiting error ($\eta \rightarrow \infty$).

613 We can see that the TD error intersects the $\eta \rightarrow \infty$ line immediately before and after
 614 the singularity. Our counterexample corresponds to the second root (that is, the
 615 intersection point at higher p .) This is because that corresponds to the stationary
 616 point between the asymptote that is crushed and the error on the right that increases.

617 If our simpler derivation proved unsatisfying, we can also derive this counterexample
 618 using this fact:

$$619 \quad 0 = \frac{d}{d\eta} \hat{w}^\top w^*(\eta) = \frac{p(p - 0.715083)}{p(p - 0.714303)^2} \quad (2.18)$$

620 From this, we can easily see that the counterexample is at $p = 0.715083$. And this
 621 completes the example! We have discovered some p at which the TD error is always
 622 at least $\|V\|$, regardless of regularization, and so our example learns a vacuous value
 623 function.

624 ***Breaking the Deadly Triad and our counterexample.***

625 In light of our example we examine the work of [62] in which the authors derive a
 626 bound for the regularized TD error under a novel double-projection update rule. We
 627 apply our example to their bound and show that their method may produce loose
 628 bounds on TD solutions, and so doesn't quite break the deadly triad:

$$629 \quad \|\Phi w^*(\eta) - V\| \leq \frac{1}{\xi} \left(\frac{\sigma_{\max}(\Phi)^2}{\sigma_{\min}(\Phi)^4 \sigma_{\min}(D)^{2.5}} \cdot \|V\| \eta + \|\Pi_D V - V\| \right) \quad (2.19)$$

for $\xi \in [0, 1]$, where σ_{\max} and σ_{\min} denote the largest and smallest singular value
 630 respectively. Theorem 2 from [62] bounds η , and therefore also b :

$$631 \quad \eta > \arg \inf_{\eta} \|\Phi - C_0\| = 0.177/(1 - \xi)^2 \quad (2.20)$$

$$632 \quad \inf_{\xi} b(\xi, \eta) = 5.20 \times 10^4 \approx 2000 * \|V\| \quad (2.21)$$

633 Their method bounds the error in our example by $2000 * \|V\|$, which is tremendously
 634 loose.

635 Analyzing the second example in 2.3.1; starting from Equation 2.19:

$$636 \quad \|\Phi w^*(\eta) - V\| \leq b(\eta, \xi) = \frac{1}{\xi} \left(\frac{\sigma_{\max}(\Phi)^2}{\sigma_{\min}(\Phi)^4 \sigma_{\min}(D)^{2.5}} \cdot \|V\| \eta + \|\Pi_D V - V\| \right) \quad (2.22)$$

$$637 \quad = 1/\xi \cdot (38.0\eta + 8.07 \times 10^{-5}) \quad (2.23)$$

for $\xi \in [0, 1]$, where σ_{\max} and σ_{\min} denote the largest and smallest singular value
638 respectively. Theorem 2 from [62] bounds η , and therefore also b :

$$639 \quad \eta > \arg \inf_{\eta} \|\Phi - C_0\| = 0.367(6.86 - 13.7\xi + 6.86\xi^2)^{-1} \quad (2.24)$$

$$640 \quad \inf_{\xi} b(\xi, \eta) = 13.8 = 7.86 * \|V\| \quad (2.25)$$

641 Under our example, their method bounds the error at no more than $7.86 * \|V\|$, which
642 is a very loose bound that permits vacuous solutions. This illustrates the risk of
643 trying to regularize away singularities, particularly in theoretical work.

644 Investigating the cause of the loose bounds reveals that the presence of $\sigma_{\min}(D)^{2.5}$
645 in 2.19 is largely responsible. As D is a diagonal matrix encoding the sampling
646 distribution, $\sigma_{\min}(D)$ is the smallest sampling rate of any state, and so the bound
647 must be at least $\frac{\eta}{\xi n^{2.5}}$ for any perfectly representable n -state MP. Unfortunately, this
648 appears to be fundamental limit caused by finding a linear bound to an error that
649 scales non-linearly, and following their derivation in the appendix does not readily
650 admit a way to improve this.

651 **2.3.2 Small amounts of regularization can cause large in-** 652 **creases in training error.**

653 There is a general assumption in the literature that ℓ_2 regularization monotonically
654 shrinks the learned weights. While this is true in classification, regression, and other
655 non-bootstrapping contexts, this is not true in TD. Because TD bootstraps values, it
656 is possible for model bias to be arbitrarily magnified.

657 This can be understood in terms of the eigenvalues of the matrix A in Equation 2.6.

658 By increasing values along the diagonal, ℓ_2 regularization increases eigenvalues of
 659 the matrix $(A + \eta I)$ to ensure it is positive definite. Under off-policy distributions,
 660 it is possible for A to have eigenvalues that are negative or zero. This implies that
 661 there are η for which $\det(A + \eta I) = 0$, and selecting η close to these values allows us
 662 to achieve arbitrarily high error. We show one such case in Example 2. This is not
 663 merely theoretical—we demonstrate this in the neural network case in Section 2.3.4.

664 **Example 2.** When TD is regularized, the model may diverge around (typically
 665 small) values of η . Lower-bounding η , a common mitigation, can make well-behaved
 666 models vacuous. It is not always possible to select a single value of η that makes
 667 models vacuous at different sampling distributions.

668 *Details.* Using our three-state example, we set $\mu = [0.05, 0.05, 0.9]$ and solve for
 669 $\det(A + \eta I) = 0$:

$$670 \quad 0 = \det(A + \eta I) = \eta^2 + 5.45 \times 10^{-2}\eta - 7.47 \times 10^{-3} \quad \implies \quad \eta = 0.0634 \quad (2.26)$$

671 As in the introductory example, the error can be made arbitrarily large by setting
 672 $\eta \approx 0.0634$. □

673 The same analysis is repeated for our second example in 2.3.1. We set $p = 0.9$ and
 674 solve for $\det(A + \eta I) = 0$:

Details.

$$675 \quad 0 = 100\eta^2 + 47.4p\eta + 1.85\eta - 1.30p^2 + 0.927p \quad (2.27)$$

$$676 \quad \eta = 0.00482577 \quad \vee \quad \eta = -0.45 \quad (2.28)$$

677 Note that the denominator of $g(p, \eta)$ is proportional to $\det(A + \eta I)$, and so $g(0.9, \eta)$ –
 678 and the error at the TD fixed point–can be made arbitrarily large by selecting η close
 679 to 4.83×10^{-3} . As this is the only positive root, the model does not diverge at other
 680 values. □

681 This small- η divergence effect can appear in several ways, illustrated in Figure 2.4a.

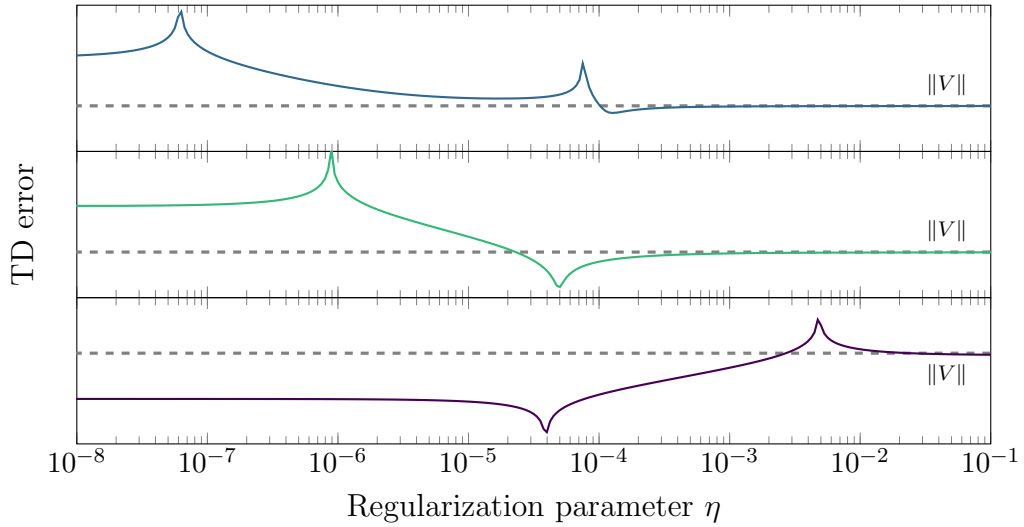
682 Typically, this appears as one or more points at which TD error diverges before the
683 region at which regularization reduces the model error below $\|V\|$. The first and
684 second plot in Figure 2.4a show two such cases, where the error increases sharply at
685 two and one points respectively.

686 In the literature, it is commonly assumed that A is “nearly” positive definite, where
687 only a few eigenvalues are non-positive, and those are close to zero. This gives rise to
688 the common mitigation of setting a lower-bound η_0 such that $(A + \eta I)$ is positive
689 definite for $\eta > \eta_0$. This may render an otherwise well-behaved model vacuous. The
690 third plot in Figure 2.4a illustrates this: the model is not vacuous when unregularized,
691 but is vacuous in the domain $\eta > 10^{-2}$ where divergence is prohibited.

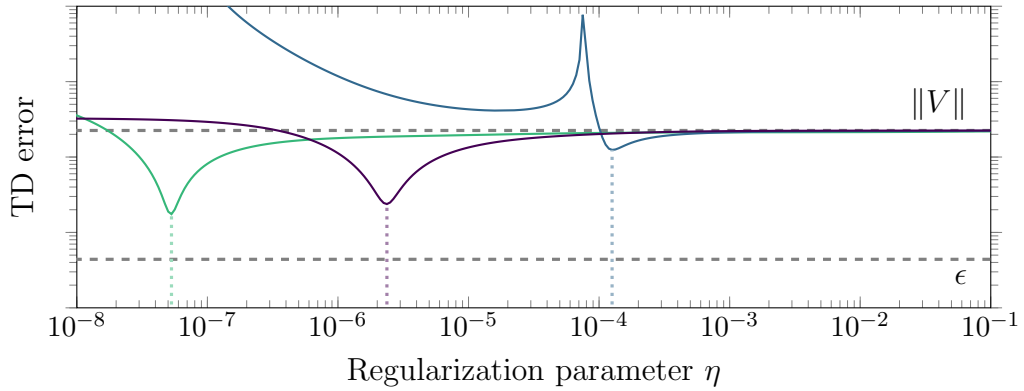
692 A common practice in the literature is to set η before training, without regard for
693 the sampling distribution. This is ill advised, as the value may be under- or over-
694 regularizing depending on the sampling distribution. One such example is illustrated
695 in Figure 2.4b, where selecting an η that minimizes the error for one distribution
696 will lead to vacuous or nearly-vacuous results in the other two. A second example in
697 Figure 2.2b has no single η for which trajectories 2 and 3 are both non-vacuous. This
698 is especially relevant as regularization is commonly used to permit distribution drift
699 during training, as discussed in Section 2.4. If the training distribution changes while
700 η is fixed, then algorithms that can be proven to converge to good solutions under
701 some original distribution may converge to poor solutions as the distribution drifts.

702 **2.3.3 Emphatic approaches and our counterexample**

703 Emphatic-TD eliminates instability from off-policy sampling by reweighing incoming
704 data (via an importance function) so it appears to be on-policy. There is considerable
705 interest in making this more practical, especially by learning the importance and
706 value models simultaneously. A leading example of this work is COF-PAC [63],
707 which uses ℓ_2 -regularized versions of GTD2 [50] to learn both the value and emphasis
708 models. The authors rely on regularization, particularly because the target policy
709 changes during learning. This makes COF-PAC vulnerable to regularization-caused



(a) Different MPs at off-policy distributions selected to show small- η error. The error may increase at multiple η , and may even occur *after* the optimal η .



(b) Three off-policy distributions with mutually incompatible η . There is no η at which all models are not vacuous or nearly vacuous.

Figure 2.4: We plot TD error against η to show small- η errors (above) and mutually-incompatible η (below). We also plot the error at the limit of vacuity $\|V\|$ and the representation error ϵ .

710 error. We illustrate this with Example 3 in which COF-PAC learns correctly when
711 unregularized, but has large error when regularized.

712 **Example 3.** COF-PAC may learn the value function with low error when unregular-
713 ized, but with arbitrarily high error when regularized.

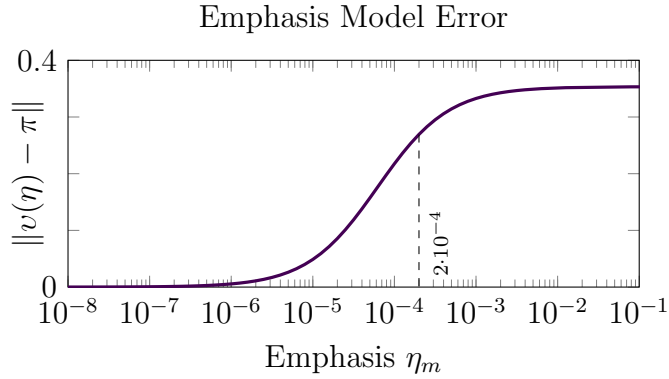
714 *Details.* Conceptually, COF-PAC maintains two separate models that are each up-
715 dated by TD: the emphasis and the value models. This emphasis model is used to
716 reweigh TD updates to the value function so they appear to come from the on-policy
717 distribution. Our strategy is to first show how regularization biases the emphasis
718 model, and then how this bias causes the value model to diverge. We begin with our
719 three-state MP, noting its on-policy distribution is $\pi = [.25 \ .25, \ .5]$. We wish to learn
720 the values using COF-PAC while sampling off-policy at $\mu = [.2 \ .2 \ .6]$.

721 Now we introduce a key conceptual tool: $v(\eta_m)$, which is the effective distribution
722 seen by the TD-updates, influenced by the emphasis regularization parameter η_m .
723 Unregularized, COF-PAC is able to resample off-policy updates to the on-policy
724 distribution: $v(0) \equiv \pi$. If the model is regularized, then the effective distribution
725 moves away from π . Figure 2.5a illustrates the distance between $v(\eta_m)$ and π as the
726 regularization parameter increases.

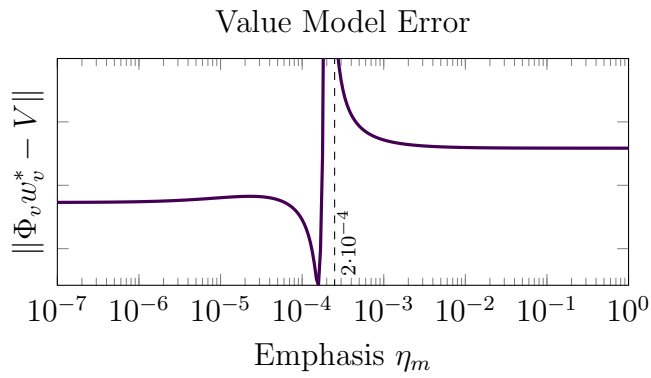
727 We can use the effective distribution to compute the error in the value model. Plotting
728 the relationship between the value function error and η_m in Figure 2.5b, we can see
729 the value function has asymptotic error around $\eta_m = 2 \times 10^{-4}$. This shows how
730 COF-PAC may diverge with specific regularization.

731 COF-PAC also allows for the value function to be separately regularized with param-
732 eter η_v . We show the effect of this in Figure 2.5c, where the value function never does
733 much better than $\|V\|$ making it (nearly) vacuous. We can conclude that regularizing
734 the emphasis model may cause the value model to diverge, and this cannot be fixed
735 by regularizing the value function separately. \square

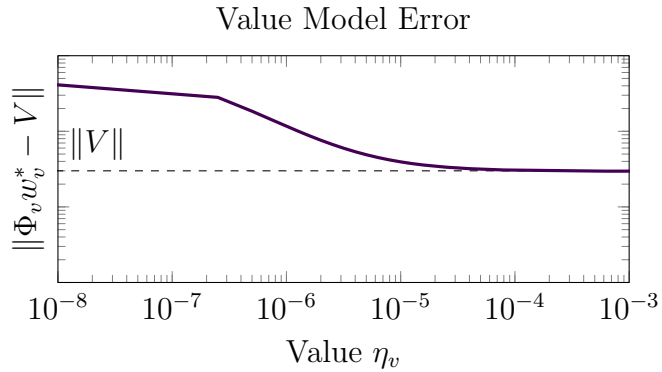
736 **Mathematical details of example.** We use an MP with the same transition
737 function as in Figure 2.1a, with separate bases Φ_m and Φ_v for the emphasis and value



(a) η_m distorts the emphasis model.

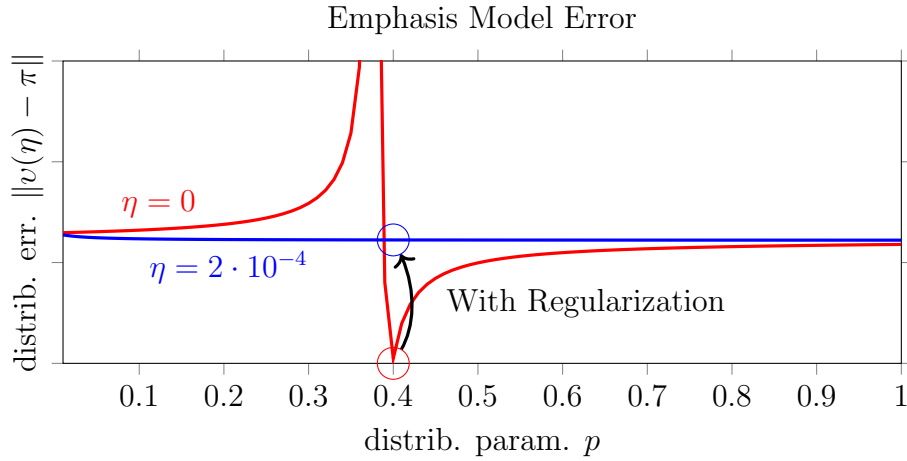


(b) η_m distorts value.

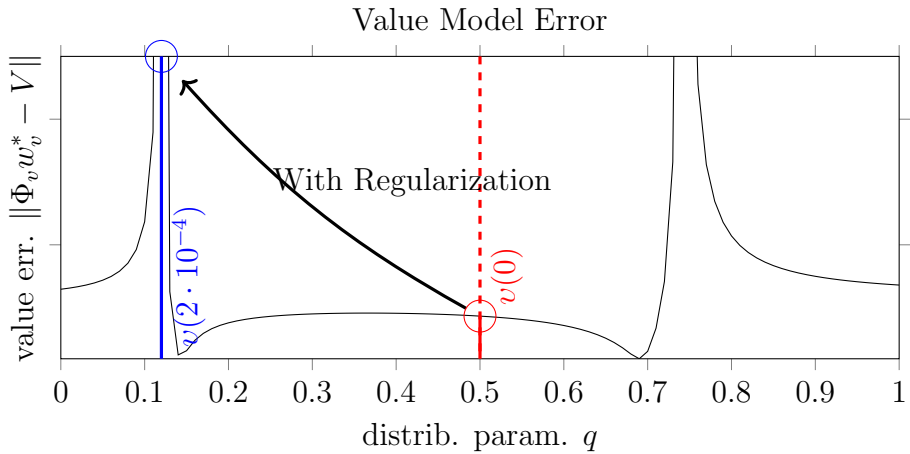


(c) η_v can't fix this.

Figure 2.5: Regularization on the emphasis model (η_m) distorts the effective distribution (Figure 2.5a). Specific values of η_m induce the value function to diverge (Figure 2.5b). The resultant value function is vacuous (Figure 2.5c). Under COF-PAC, regularization can greatly increase model error.



(a) distribution is $[p/2, p/2, (1 - p)]$



(b) distribution is $[(1 - q)/2, q/2, 0.5]$

Figure 2.6: Regularization distorts the emphasis model (left), which induces the value function (right) to move to a singularity. Unregularized models are shown in red, regularized models in blue. Regularization can interact with emphasis models to significantly worsen learned value functions.

738 stages respectively. We assume that our interest in all states is uniformly $i = 1$.

739 We begin by setting the off-policy sampling distribution of $\mu = [.2 \ .2 \ .6]$, used as the
 740 diagonal matrix $D_\mu = \text{diag}(\mu)$. Thanks to the simple structure of our example, we
 741 know the emphasis is $m = \frac{i}{1-\gamma} \cdot \pi D_\mu^{-1} \propto (5/4, 5/4, 5/6)$. We select a basis that allows
 742 us to represent this emphasis:

$$743 \quad \Phi_m = \begin{bmatrix} 5/4 & 0 \\ 0 & -1/100 \cdot 5/4 \\ 5/12 & -1/100 \cdot 5/12 \end{bmatrix} \quad (2.29)$$

We deliberately choose Φ_m to have a poor condition number for reasons that will
 744 become apparent later. We can represent $c \cdot (5/4, 5/4, 5/6)$ exactly for any constant c :

$$745 \quad \Phi_m \cdot (1, -100) \cdot c = c \cdot (5/4, 5/4, 5/6) \quad (2.30)$$

746 Using Equation 5 from [63], we define the matrices:

$$747 \quad C_m = \Phi_m^\top D_\mu \Phi_m = \begin{bmatrix} 0.417 & -1.04 \times 10^{-3} \\ -1.04 \times 10^{-3} & 4.17 \times 10^{-5} \end{bmatrix} \quad (2.31)$$

$$748 \quad A_m = \Phi_m^\top (I - \gamma P^\top) D_\mu \Phi_m = \begin{bmatrix} 0.159 & 1.536 \times 10^{-3} \\ 1.536 \times 10^{-3} & 1.59 \times 10^{-5} \end{bmatrix} \quad (2.32)$$

And we apply these to the formulation in Lemma 3 and compute the emphasis weights
 749 as a function of the regularization $w_m : \mathbb{R}_0^+ \rightarrow \mathbb{R}^+$:

$$750 \quad w_m^*(\eta) = (A_m^\top C_m^{-1} A_m + \eta I)^{-1} A_m^\top C_m^{-1} \Phi_m^\top D i \quad (2.33)$$

751 We can then use this to compute the new apparent distribution v , which is the
 752 effective distribution that the updates to the value model see, and it is equal to the

753 emphasis multiplied by the off-policy distribution.

$$754 \quad v(\eta) = \Phi_m \cdot w_m^*(\eta) \cdot D \quad (2.34)$$

755 Without any regularization, this should be exactly equal to the on-policy distribution.

$$756 \quad v(0) = [0.25 \ 0.25 \ 0.5] \equiv \pi \quad (2.35)$$

When we compute this value with a small amount of regularization $\eta = 2 \times 10^{-4}$, we
757 observe that the apparent distribution drifts far away from the on-policy distribution.

$$758 \quad v(2 \times 10^{-4}) = [0.44 \ 0.06 \ 0.5] \quad (2.36)$$

759 The proximate cause of this is the poor condition number of C , caused by the $\frac{1}{100}$
760 scale factor applied to the second column of Φ_m . This allows η to affect different
761 columns by different (relative) amounts in the definition of $w^*(\eta)$, which pushes it
762 away from the symmetric solution. See this error shift in Figure 2.6a.

763 So far, we have shown how regularization causes a shift in the apparent distribution
764 that the TD updates see. To complete the example we show how this moves the
765 fixed point of the value function away from a stable point into an asymptote where it
766 may grow without bounds. This second phase follows in the same pattern as the first
767 phase, starting with the desired value function: $V = [1 \ 2.69 \ 1.05]$ and a basis that
768 can almost exactly represent the value function:

$$769 \quad \Phi_v = \begin{bmatrix} 1 & 0 \\ 0 & -2.69 \\ 1/2(\epsilon + 1.05) & -1/2(\epsilon + 1.05) \end{bmatrix} \quad (2.37)$$

$$770 \quad \epsilon = 2 \times 10^{-4} \quad (2.38)$$

We use this basis to compute the state-rewards $R = (I - \gamma P)V = [-0.43 \ 1.26 \ -0.38]$
 771 and define the matrices A_v and C_v and the solution $w_v^*(\eta)$:

$$772 \quad A_v = \Phi_v^\top (I - \gamma P^\top) D \Phi_v \quad (2.39)$$

$$773 \quad C_v = \Phi_v^\top D \Phi_v \quad (2.40)$$

$$774 \quad w_v^*(\eta) = (A_v^\top C_v^{-1} A_v + \eta I)^{-1} A_v^\top C_v^{-1} \Phi_v^\top D R \quad (2.41)$$

We can use this solution to compute the error between the value function and the true
 values, $\|\Phi_v w_v(\eta) - V\|$. First, under the corrected distribution without regularization
 775 $v(0) \equiv \pi$:

$$776 \quad \Phi_v w_v^*(0)|_{D=\text{diag}(v(0))} = 0.000865 \quad (2.42)$$

777 Then, with regularization in the value function (but not in the emphasis function):

$$778 \quad \Phi_v w_v^*(2 \times 10^{-4})|_{D=\text{diag}(v(0))} = 0.0162 \quad (2.43)$$

Then, under the apparent distribution v induced by use of regularization in the
 779 emphasis function, without and with regularization:

$$780 \quad \Phi_v w_v^*(0)|_{D=\text{diag}(v(2 \times 10^{-4}))} = 418.601 \quad (2.44)$$

$$781 \quad \Phi_v w_v^*(2 \times 10^{-4})|_{D=\text{diag}(v(2 \times 10^{-4}))} = 3.00 \quad (2.45)$$

782 It is immediately obvious that the use of regularization in the emphasis function
 783 causes the learned value function to be incorrect. Including a regularizing term in the
 784 value estimate is not sufficient to fix the value function. This completes the example.

785 **The non-expansion condition and our counterexample.**

786 COF-PAC makes the strong assumption that Kolter's non-expansion condition [24,
 787 eqn. 10] holds in both the emphasis and value models [63, asm. 4]. This is itself
 788 a very strong condition because it inherently assumes that both the emphasis and

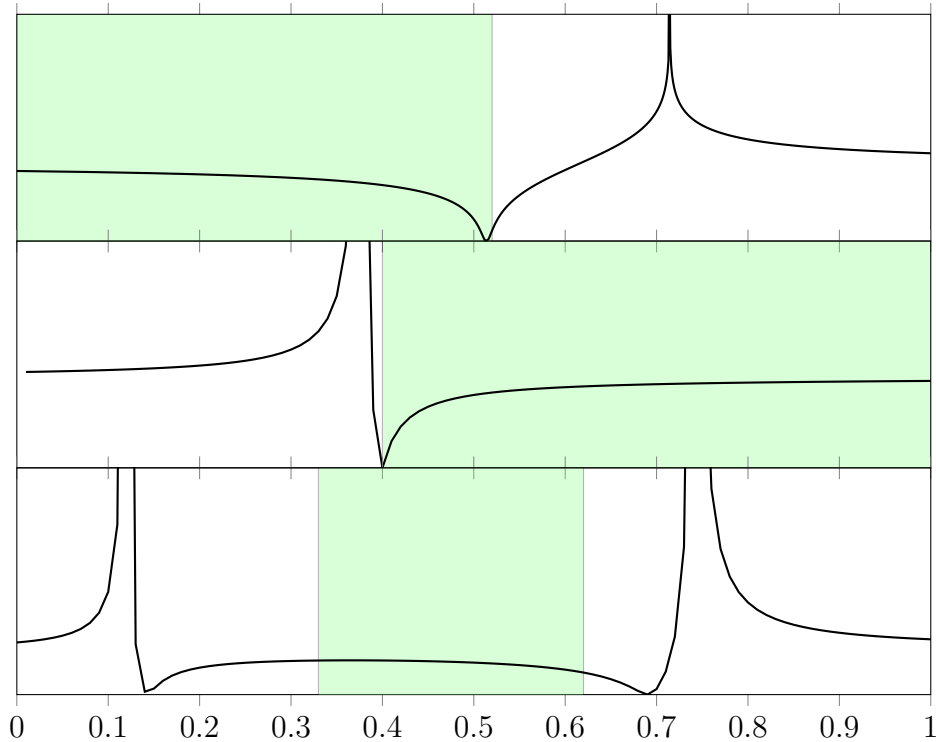


Figure 2.7: The non-expansion condition holds in the shaded region of each graph. These correspond to Figure 2.3, Figure 2.6a, and Figure 2.6b respectively.

789 value models are not subject to runaway TD [63, asm. 4]. Specifically, they make
 790 the strong assumption that this condition [24, eqn. 10] holds in the emphasis model
 791 at μ and value model at v . This condition selects a convex subset of distributions
 792 under which one-step transition followed by projection onto Φ is non-expansive. We
 793 illustrate these regions in Figure 2.7. Even in the one-dimensional parameterization
 794 shown, this condition only holds in a small sub-region of the space and therefore
 795 appears to be a very strong condition. Empirically determining if such a condition
 796 holds (or training models to enforce it) may be possible with TD-DO [24, sec 4.1],
 797 but it is not clear how that method interacts with regularization.

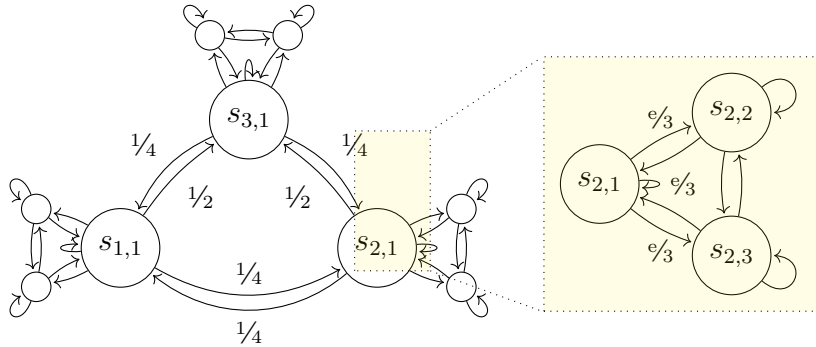


Figure 2.8: Our three-state counter-example MP is extended to nine states to illustrate how the deadly triad problem could manifest in multi-layer neural networks. The self-loop in the original example is replaced with a clique with uniform transitions except as labelled with the original edge weight e .

$$\frac{1}{12} \begin{bmatrix} 1 & 1 & 1 & 3 & & 6 \\ 4 & 4 & 4 & & & \\ 4 & 4 & 4 & & & \\ 3 & & & 1 & 1 & 1 & 6 \\ & & & 4 & 4 & 4 & \\ & & & 4 & 4 & 4 & \\ 3 & & & 3 & & & 2 & 2 & 2 \\ & & & & & & 4 & 4 & 4 \\ & & & & & & 4 & 4 & 4 \end{bmatrix}$$

(a) Transition function of the MDP.

(b) Observation function of the MDP.

Figure 2.9: Our three-state counterexample Markov Process. We use this to illustrate how TD models can fail despite common mitigating strategies with linear function approximation.

798 2.3.4 Applied to multi-layer networks

799 We use a 9-state variant of our example to study the deadly triad in multi-layer neural
800 networks (NNs). The MDP and its transition function are depicted in Figure 2.9; we
801 have transformed the original MDP by replacing each self-loop with two additional
802 states, forming a clique with the original state. We also define a deterministic
803 observation function $o : \mathcal{S} \rightarrow \mathbb{B}^6$, where each state is encoded as the concatenation of
804 the one-hot vector of its subscripts. The value function is assigned pseudo-randomly
805 in range $[-1, 1]$, and a consistent reward function is assigned. We select the family
806 of sampling distributions $\mu \propto [4p, 1p, 1p, 4p, 1p, 1p, 8(1-p), 4(1-p), 4(1-p)]$,
807 where the on-policy distribution is at $p = 0.5$.

808 We train a simple two-layer neural network with 3 neurons in the hidden layer. The
809 value function is assigned pseudo-randomly in range $[-1, 1]$.

810 **Example 4.** Vacuous models and small- η error also occur in neural network condi-
811 tions.

812 *Details.* We train 100 models using simple semi-gradient TD updates under a fixed
813 learning rate. We plot the mean and the 10th–90th percentile range in Figure 2.10a,
814 with and without regularization. TD is known to exhibit high variance, and regular-
815 ization is the traditional remedy for that. We corroborate this by noting that the
816 performance of the unregularized model varies widely, but regularization leads to
817 similar performance across initializations at the cost of increased error.

818 First, we show that vacuous models may exist in the neural network case. In
819 Figure 2.10a, note how there are some off-policy distributions under which both the
820 regularized and unregularized models perform worse than the threshold of vacuity.
821 We can numerically verify that vacuous models exist. Second, we show the small- η
822 error problem in the neural network case in Figure 2.10b, where we plot the TD
823 error against η at a fixed off-policy distribution. We observe that around $\eta \approx 10^{-3}$
824 the TD Error unexpectedly *increases* before decreasing, which clearly illustrates this
825 phenomenon. \square

826 We wish to learn the model with a two-layer network with $k < n$ nodes in the inner
827 layer. We define the network as $f(o(s_{i,j})) = \tan^{-1}(o(s_{i,j}) * \omega_1) * \omega_2$. The parameters
828 $\omega_1 \in \mathbb{R}^{6 \times k}$, $\omega_2 \in \mathbb{R}^{k \times 1}$ are trained to convergence using simple TD updates with
829 semi-gradient updates, a fixed learning rate, and without a target network.

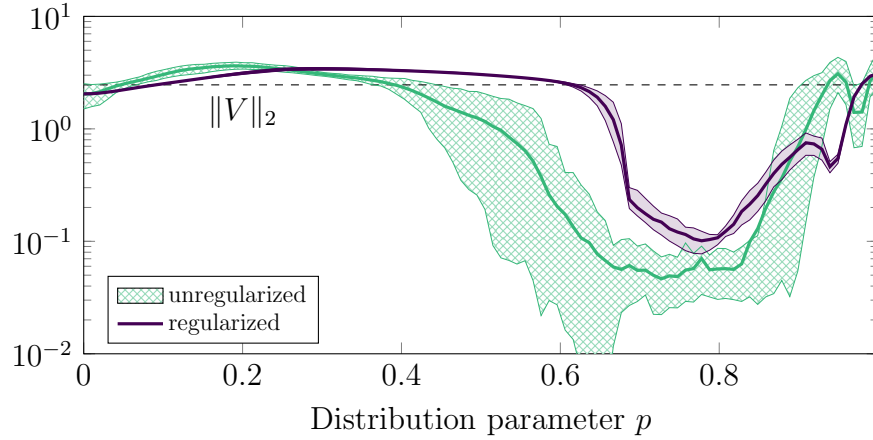
830 In addition to the example in Figure 2.10b, we present an additional example in
831 Figure 2.11. The same Markov process, at a different off-policy distribution, attains
832 a curve where the non-vacuous region lies before the divergent region, similar to
833 the second row in Figure 2.4a. An added observation is that these two graphs are
834 mutually incompatible – there is no fixed η that can simultaneously do better than
835 vacuity in both, which promotes the idea of testing multiple regularization parameters
836 or using an adaptive regularization scheme.

837 **2.3.5 Over-parameterization does not solve this problem**

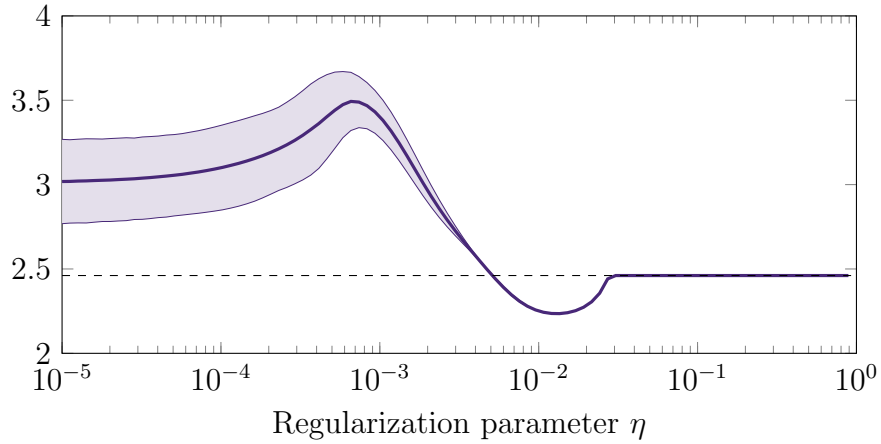
838 Baird’s counterexample [58] shows how, in the linear case, that off-policy divergence
839 can also happen with over-parameterization, as long as some amount of function
840 approximation occurs. It is not obvious that this conclusion persists in the neural
841 network case, so we include an additional example showing that the parameterization
842 doesn’t resolve small- η divergence.

843 In Figure 2.12 we plot models with 3 to 13 nodes in the hidden layer. For reference,
844 the MDP has 9 states, so some models under-parameterize and some models over-
845 parameterize. We observe that, in the low-regularization regime, increasing the
846 number of parameters improves the error slightly. However, increasing the number
847 of parameters in the hidden layer does not change the behavior in the the small- η
848 divergence region.

849 These qualitative links show a clear connection between the neural network case
850 and the linear case, and highlights the importance of correctly handling off-policy
851 sampling.



(a) Mean and 10th–90th percentile errors of 100 NN value models trained to convergence.



(b) The relationship between error and η at the off-policy distribution $p = 0.31$.

Figure 2.10: We illustrate how regularization interacts with NN value functions, showing that the problems identified in this chapter persist in the NN case.

852 2.4 Related Work

853 Three examples of the deadly triad are common in the literature: the classic
854 Tsitsiklis and Van Roy ($w, 2w$) example [48, p. 260], Kolter’s example [24], and
855 Baird’s counterexample which shows how training instability can exist despite over-
856 parameterization [58].

857 ℓ_2 regularization is common when proving that an algorithm converges under a
858 changing sampling policy. This is seen in GTD (analyzed in [60]), GTD2 [50], RO-
859 TD [33], and COF-PAC [63]. This assumption may also be used to ensure convergence
860 when training with a target network [62]. Despite the prevalence of regularization, the
861 induced bias from using it is not well studied. It is often dismissed as a mere technical
862 assumption, as in [8]. We contradict that: using regularization for convergence proofs
863 may induce catastrophic bias. By showing concrete examples, this work hopes to
864 inspire further investigation into regularization-induced bias in the same vein as [60].

865 **Alternatives to regularization and TD** We focus on ℓ_2 regularization in this
866 chapter, which penalizes the ℓ_2 -norm of the learned weights; it is also possible to
867 use ℓ_1 regularization with a proximal operator/saddle point formulation as in [33],
868 or any convex regularization term under a fixed target policy [60]. Instead of
869 directly regularizing the weights, COP-TD uses a discounted update [13]. DisCor [25]
870 propagates bounds on Q-value estimates to quickly converge TD learning in the
871 face of large bootstrapping error; it is not clear if DisCor can overcome off-policy
872 sampling. A separate primal-dual saddle point method has also been adapted to ℓ_2
873 regularization [9] and is known to converge under deadly triad conditions, and recent
874 work [56] has derived error bounds with improved scaling properties in the linear
875 setting, offering a promising line of research.

876 Emphatic-TD [49] fixes the fundamental problem in off-policy TD by reweighing
877 updates so they appear on-policy. The core idea underlying these techniques is to
878 estimate the “follow-on trace” for each state, the (weighted, λ - and γ -discounted)
879 probability mass of all states whose value estimates it influences. This trace is then

880 used to estimate the emphasis, which is the reweighing factor for each update. While
881 this family of methods is provably optimal in expectation, it is subject to tremendous
882 variance in theory and practice, especially when the importance is estimated using
883 Monte-Carlo sampling.² In practice, these methods learn the follow-on trace using
884 TD [19, 63] or similar [17], which makes them vulnerable to bias induced by the use
885 of regularization.

886 2.5 Relationship to modern RL algorithms

887 It is still not obvious how strongly this instability affects modern RL algorithms,
888 which are also sensitive to a variety of other failure modes. Unlike our analysis,
889 the sampling distribution changes during training, and regularization mechanisms
890 are more complex than simple ℓ_2 penalties. The exact relationship between the
891 instabilities we study and RL algorithms is an open problem, but we offer two pieces
892 of indirect evidence suggesting there is a link.

893 First, in the offline/batch RL literature, it is well-known that online RL algorithms
894 naively applied can catastrophically fail if the learned policy is not consistent with
895 the data distribution. This is known as the distribution shift problem, [31, p. 26] and
896 offline RL algorithms are generally constructed to explicitly address this. Second,
897 when using experience replay buffers in online RL algorithms, policy quality generally
898 improves when older transitions are more quickly evicted [10]. However, there are
899 multiple factors at work here, and it is not possible to separate out the instability
900 from off-policy sampling from the remaining factors.

901 2.6 Conclusion

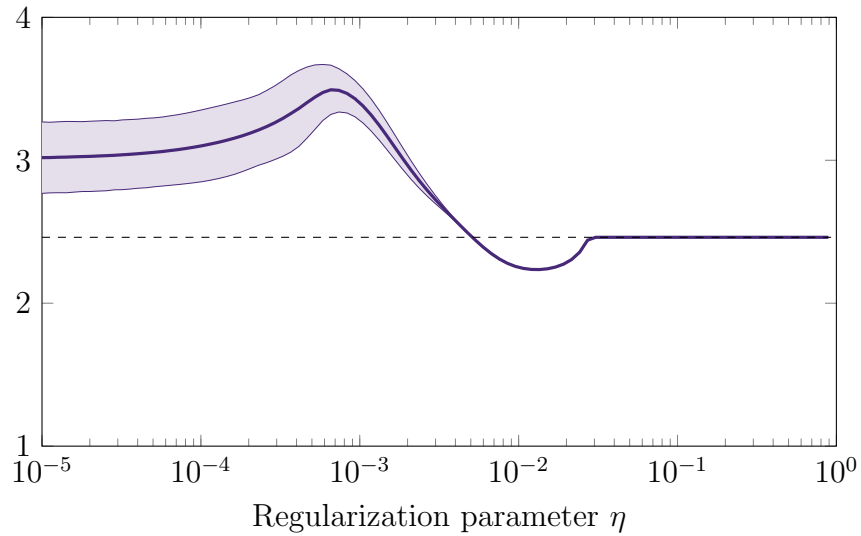
902 There is a tremendous focus in the RL literature on proving convergence of novel
903 algorithms, but not on the error at convergence. Papers like [62] are laudable

²Sutton and Barto’s textbook [48] says about Emphatic-TD that “it is nigh impossible to get consistent results in computational experiments.” (when applied to Baird’s example).

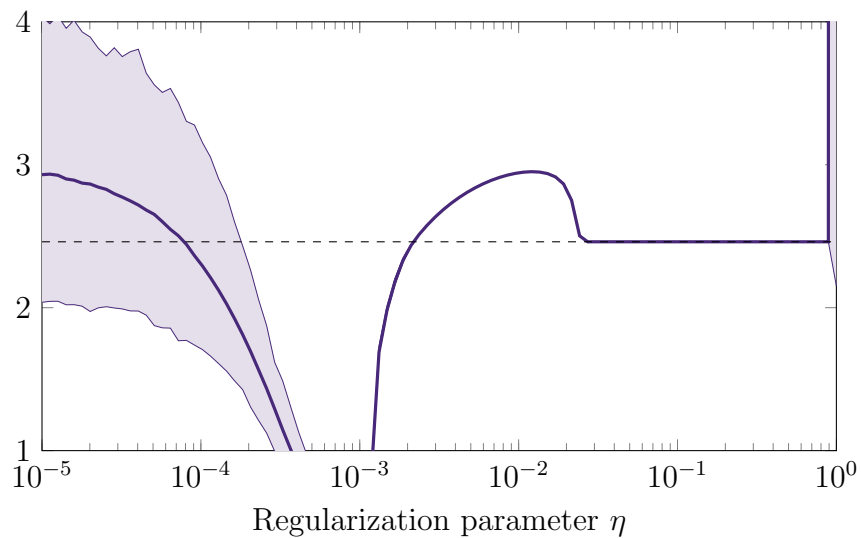
904 because they provide error bounds; even if the current bounds are loose, future
905 work will no doubt tighten them. In this work, we show that the popular technique
906 of ℓ_2 regularization does not always prevent singularities and could even introduce
907 catastrophic divergence. We show this with a new counterexample that elegantly
908 illustrates the problems with learning off-policy and how it persists into the NN case.

909 Even though regularization can catastrophically fail in the ways we illustrate, it
910 remains a reasonable method that may offer a fair tradeoff—as long as we are careful
911 to check that we are not running afoul of the failure modes we explain here. It may be
912 possible to design an adaptive regularization scheme that can avoid these pathologies.
913 For now, testing the model performance over a range of regularization parameters
914 (spanning several orders of magnitude) is the best option we have to detect such
915 pathological behavior.

916 Emphatic-TD is perhaps the most promising area of research for mitigating off-policy
917 TD-learning. The key problem preventing its widespread adoption is the difficulty
918 in estimating the emphasis function, but future work in this area may be able to
919 overcome this. Our example shows the risk of relying on regularization in practical
920 implementations of such methods. It is absolutely critical that Emphatic algorithms
921 correctly manage regularization to avoid the risks that we highlight here.

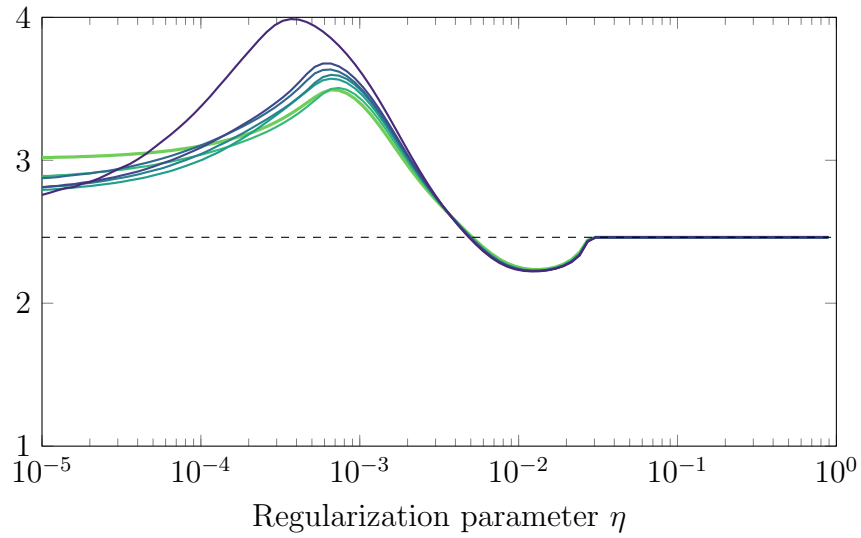


(a) $p = 0.31$ (From Figure 2.10b)

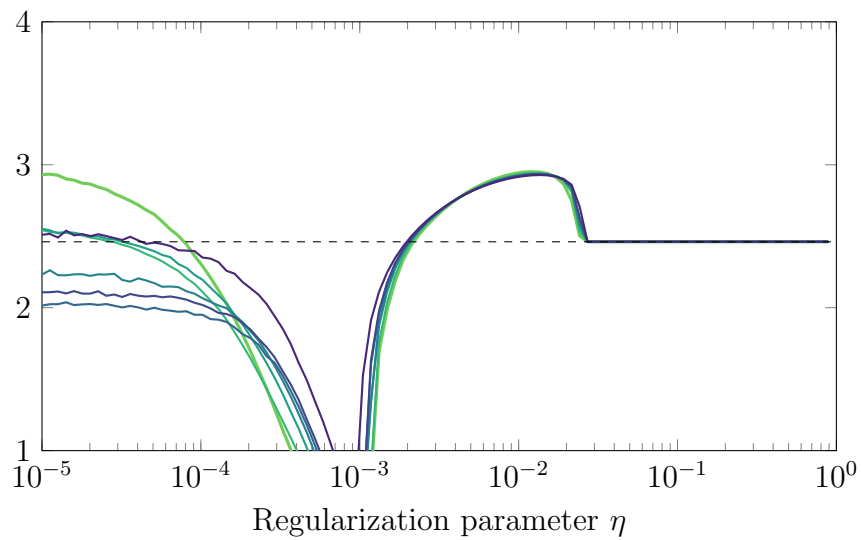


(b) $p = 0.95$

Figure 2.11: The relationship between error and η at different off-policy distributions, showing mutually incompatible regularization behavior. The shaded range indicates the region between the 5th and 95th percentile of 100 differently-initialized models.



(a) $p = 0.31$



(b) $p = 0.95$

Figure 2.12: The relationship between η and error with different amount of model parameterization (with 3, 5, 7, 9, 11, 13, and 64 nodes in the hidden layer, corresponding to darkening colors.)

922 Chapter 3

923 Projected Off-Policy TD for Offline 924 Reinforcement Learning

925 A key problem in offline Reinforcement Learning (RL) is the mismatch between the
926 dataset and the distribution over states and actions visited by the learned policy,
927 called the *distribution shift*. This is typically addressed by constraining the learned
928 policy to be close to the data generating policy, at the cost of performance of the
929 learned policy. We propose Projected Off-Policy TD (POP-TD), a new critic update
930 rule that resamples TD updates to allow the learned policy to be distant from the
931 data policy without catastrophic divergence. We show how this algorithm works
932 on a well-understood toy example from the literature, and then characterize its
933 performance with varying parameterization on a specially-constructed offline RL task.
934 This is a novel approach to stabilizing off-policy RL, and sets the stage for future
935 work on larger tasks.

936 *Paper in preparation, by Manek, Roderick, and Kolter (2023)*

937 3.1 Introduction

938 Reinforcement Learning (RL) aims to learn policies that maximize rewards in Markov
939 Decision Processes (MDPs) through interaction, generally using Temporal Difference
940 (TD) methods. In contrast, offline RL focuses on learning optimal policies from a
941 static dataset sampled from an unknown policy, possibly a policy designed for a
942 different task. Thus, algorithms are expected to learn without the ability to interact
943 with the environment. This is useful in environments that are expensive to explore
944 (such as running a Tokamak nuclear reactor [7]), or high-dimensional environments
945 with cheap access to expert or near-expert trajectories (such as video games). Levine
946 et al. [30] present a comprehensive survey of the area.

947 Since in offline RL the data is gathered before training begins, there is a mismatch
948 between the the state-distributions implied by the learned policy and the data. When
949 applying naive RL algorithms in this setting, they tend to bootstrap from regions
950 with little or no data, causing runaway self-reinforcement. Offline RL algorithms
951 like Conservative Q-Learning (CQL) [26], on the other hand, generally constrain the
952 learned policy to remain within the support of the data. While this works well in
953 practice, there still remains a large gap in performance between online and offline
954 RL. One reason for this is an additional subtlety to distribution shift: because of the
955 combination of off-policy RL and function approximation, it is possible for RL to
956 diverge if the generating policy and the learned policy are sufficiently different.

957 We illustrate a simple case in Figure 3.1, where a simple grid environment is designed
958 to elicit the shortest trajectory from start (S) to goal (G). Agents can move one step
959 in each cardinal direction, reaching the goal yields a unit reward, and the episode
960 ends on reaching the goal or any marked cell (X). We generate a dataset by following
961 a suboptimal data policy (•••) with sufficient dithering to guarantee that every state-
962 action pair is represented. If we use a tabular Q-function, we can recover the optimal
963 policy (—) and obtain the true value function. When we use a linear Q-function,
964 however, the error is much larger. We find that about half of random initializations
965 lead to Q-functions that either diverge or converge to large error. This shows how

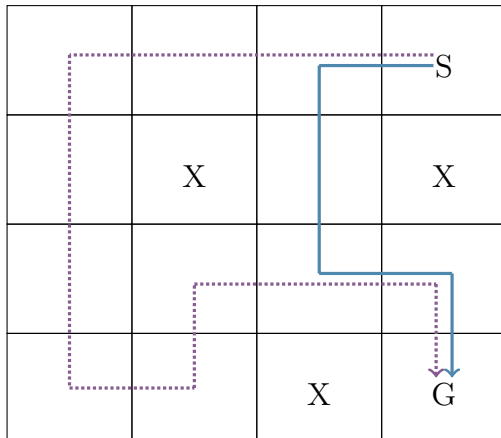


Figure 3.1: A simple grid environment illustrating distribution shift despite complete support. We wish to learn the optimal trajectory (—) from a suboptimal data policy (---) which is ϵ -dithered to get sufficient coverage. When we apply Q-learning methods to this, training often diverges to arbitrarily poor values. This is a consequence of distribution shift. In this paper, we propose a technique to solve this divergence.

966 even with full coverage of states and actions, distribution shift can be a significant
 967 source of error. We provide more details in Section 3.5.1.

968 **Contributions** In this chapter, we introduce POP-TD, a novel method of mitigating
 969 the error from off-policy learning. We show theoretically that this method bounds the
 970 off-policy approximation error for TD-based RL methods. We illustrate the resampling
 971 process on a well-known toy example, and then demonstrate its effectiveness on an
 972 example of offline RL under distribution shift.

973 3.2 Related Work

974 **Off-Policy TD Learning** Instability from learning off-policy has also been studied
 975 in the classic RL literature. First described by Tsitsiklis and Van Roy [53], the use
 976 of TD learning, function approximation, and off-policy sampling may cause severe
 977 instability or divergence. This is known as the *deadly triad* [48, p. 264] and even if

978 many variants of TD still converge, the quality of the solution at convergence may be
979 arbitrarily poor [24].

980 There are three existing lines of work in the literature that attempt to resolve this:
981 regularization, Emphatic reweighing, and TD Distribution Optimization (TD-DO).
982 The first attempts to regularize TD, typically with \mathcal{L}_2 -norm weight regularization.
983 Alternative regularization schemes are \mathcal{L}_1 [33], convex [60], and bounds propagation
984 [25]. There are well-documented failure modes related to regularization [35]. The
985 second line started with Emphatic-TD, in which Sutton, Mahmood, and White [49]
986 note that it is possible to reweigh samples obtained off-policy so they appear to be
987 on-policy. Such methods learn the follow-on trace using Monte-Carlo methods (in the
988 original), TD [19, 63] or techniques similar to TD [17]. The third method, TD-DO,
989 works by solving a small optimization problem on each TD update to reweigh samples
990 to satisfy the Non-Expansion Criterion, which we introduce in the next section.

991 **Off-Policy and Offline Deep RL** Nearly all modern TD-based deep RL methods
992 perform off-policy learning in practice. To improve data efficiency and learning
993 stability, an experience replay buffer is often used. This buffer stores samples from
994 an outdated version of the policy [38]. Additionally, exploration policies, such as a
995 epsilon greedy [48, p. 100] or Soft Actor Critic (SAC)-style entropy regularization [15]
996 ¹, are often used, which also results in off-policy learning. In practice, the difference
997 between the current policy and the samples in the buffer is limited by setting a limit to
998 the buffer size and discarding old data; or by keeping the exploration policy relatively
999 close to the learned policy. In practice, this is sufficient to prevent outright divergence,
1000 though the extent to which it decreases performance is not well-understood.

1001 However, in the offline RL setting where training data is static, there is usually a
1002 much larger discrepancy between the state-action distribution of the data and the
1003 distribution induced by the learned policy. This discrepancy presents a significant
1004 challenge for offline RL [30]. While this distributional discrepancy is often presented

¹While the original SAC algorithm is technically on-policy since it learns an entropy-regularized value function, the entropy-regularization is often dropped from the value-function estimate in practice to improve performance.

1005 as a single challenge for offline RL algorithms, there are two distinct aspects of this
 1006 challenge that can be addressed independently: *support mismatch* and *proportional*
 1007 *mismatch*. When the support of the two distributions differ, learned value functions
 1008 will have arbitrarily high errors in low-data regions. Support mismatch is dealt with
 1009 by either constraining the KL-divergence between the data and learned policies [11,
 1010 28, 59], by penalizing or pruning low-support (or high-uncertainty) actions [26, 61,
 1011 22].

1012 Even when the support of the data distribution matches that of the policy distribution,
 1013 naive TD methods can produce unbounded errors in the value function [53]. We call
 1014 this challenge *proportional mismatch*.

1015 Importance sampling (IS) [44] is one of the most widely used techniques to address
 1016 proportional mismatch. The idea with IS is to compute the differences between the
 1017 data and policy distributions for every state-action pair and re-weight the TD updates
 1018 accordingly. However, these methods suffer from variance that grows exponentially in
 1019 the trajectory length. Several methods have been proposed to mitigate this challenge
 1020 and improve performance of IS in practice [16, 13, 40, 39, 32], but the learning is still
 1021 far less stable than other offline deep RL methods. In this work, we propose a new
 1022 method to bound the value-function approximation errors caused by proportional
 1023 mismatch without the need to explicitly compute (or approximate) IS weights.

1024 3.3 Problem Setting and Notation

1025 Consider the n -state Markov chain $(\mathcal{S}, P, R, \gamma)$, with state space \mathcal{S} , transition function
 1026 $P : \mathcal{S} \times \mathcal{S} \rightarrow \mathbb{R}_+$, reward function $R : \mathcal{S} \rightarrow \mathbb{R}$, and discount factor $\gamma \in [0, 1]$. Because
 1027 the state-space is finite, it can be indexed as $\mathcal{S} = \{1, \dots, n\}$. This allows us to use
 1028 matrix rather than operator notation. The expected γ -discounted future reward of
 1029 being in each state $V(s) := \mathbb{E}[\sum_{t=0}^{\infty} \gamma^t R(s_t) | s_0 = s]$ is called the value function. The
 1030 value function is consistent with Bellman’s equation (in matrix form):

$$1031 \quad V = R + \gamma PV. \quad (3.1)$$

1032 In the linear setting, we approximate the value function as $V(s) \approx w^\top \phi(s)$, where
 1033 $\phi : \mathcal{S} \rightarrow \mathbb{R}^k$ is a fixed basis function and we estimate parameters $w \in \mathbb{R}^k$. In matrix
 1034 notation, we write this as $V \approx \Phi w$.

1035 In this work, we are interested in the offline learning setting, where the sampling
 1036 distribution μ differs from the stationary distribution ν . In this setting, the TD
 1037 solution is:

$$1038 \quad \Phi w = \Pi_\mu (R + \gamma P \Phi w), \quad (3.2)$$

1039 where $\Pi_\mu = \Phi (\Phi^\top D_\mu \Phi)^{-1} \Phi^\top D_\mu$ is the projection onto the column space of Φ weighted
 1040 by the data distribution μ through the matrix $D_\mu = \text{diag}(\mu)$. This projection may be
 1041 arbitrarily far from the true solution, and so the error may be correspondingly large.
 1042 The literature bounds the error as:

1043 **Theorem 2.** *The error at the TD fixed point is $\|\Phi w - V\|_{D_\mu}$. Lemma 6 from [53]*
 1044 *bounds this in terms of error projecting V onto the column space of Φ :*

$$1045 \quad \|\Phi w - V\|_{D_\mu} \leq \frac{1}{1 - \gamma} \|\Pi_\mu V - V\|_{D_\mu} \quad (3.3)$$

1046

1047 3.3.1 The Non-Expansion Criterion (NEC)

1048 Thus far we have left open the notion of a “safe” distribution to resample TD updates
 1049 to. The on-policy distribution must be safe, but we need to establish a criteria for
 1050 acceptable off-policy distributions. Tsitsiklis and Van Roy lay the groundwork for
 1051 this by analyzing the training of on-policy TD as a dynamical system and showing
 1052 that once TD reaches its fixed point, subsequent TD updates form a non-expansive
 1053 mapping around that fixed point (1996, lemma 4), and therefore prove that on-policy
 1054 TD does not diverge.

1055 To do this, they begin with the fact that error bounds from on-policy TD follow

1056 the property that the D -norm of any vector $x \in \mathbb{R}^n$ is non-expansive through the
 1057 transition matrix. That is: $\|Px\|_D \leq \|x\|_D$, where $D = \text{diag}(\pi)$. Kolter [24] extend
 1058 this analysis to the off-policy case, deriving a linear matrix inequality (LMI) under
 1059 which the TD updates are guaranteed to be non-expansive around the fixed point.
 1060 This is the Non-Expansion Criterion (2011):

$$1061 \quad \|\Phi w - V\|_D \leq \frac{1 + \gamma \kappa(D^{-1/2} D^{1/2})}{1 - \gamma} \|\Pi_D V - V\|_D \quad (3.4)$$

1062 From this bound, he derives *The non-expansion criterion*:

$$1063 \quad \|\Pi_D P \Phi w\|_D \leq \|\Phi w\|_D \quad (\forall w \in \mathbb{R}^n) \quad (3.5)$$

1064 This holds if and only if the matrix F_D is positive semi-definite

$$1065 \quad F_D \equiv \begin{bmatrix} \Phi^\top D \Phi & \Phi^\top D P \Phi \\ \Phi^\top P^\top D \Phi & \Phi^\top D \Phi \end{bmatrix} \succcurlyeq 0 \quad (3.6)$$

1066 Equivalently, in terms of the expectation over states:

$$1067 \quad \mathbb{E}_{s \sim \mu, s' \sim p(\cdot|s)} \left[\begin{bmatrix} \phi(s)\phi(s)^\top & \phi(s)\phi(s')^\top \\ \phi(s')\phi(s)^\top & \phi(s)\phi(s)^\top \end{bmatrix} \right] \succcurlyeq 0. \quad (3.7)$$

1068 This constraint describes a convex subset of D . As a $2k \times 2k$ matrix (where k is the
 1069 number of features), F is prohibitively large to enumerate for any real RL problem,
 1070 and so our algorithm is designed to make use of this without ever constructing it
 1071 directly. Further, we notice that the construction of F_D depends on P , the transition
 1072 matrix of the underlying Markov process, which complicates how we construct it from
 1073 samples.

1074 For convenience, we write this as:

$$1075 \quad \mathbb{E}_{s \sim q}[F(s)] \succcurlyeq 0, \text{ where} \quad (3.8)$$

$$1076 \quad F(s) = \mathbb{E}_{s' \sim p(s'|s)} \left[\begin{bmatrix} \phi(s)\phi(s)^\top & \phi(s)\phi(s')^\top \\ \phi(s')\phi(s)^\top & \phi(s)\phi(s)^\top \end{bmatrix} \right]. \quad (3.9)$$

1077 KNEC is an expectation over some state distribution q and transition distribution
 1078 $p(s, s') = p(s'|s)\mu(s)$. Because it is an LMI, the satisfying state distributions q form
 1079 a convex subset.

1080 Directly constructing $F(s)$ or $F(s, s')$ is impossible on all but the simplest examples –
 1081 it would take $\mathcal{O}(k^2n)$ or $\mathcal{O}(k^2n^2)$ memory to hold all the necessary data. Instead we
 1082 exploit the structure inherent in the problem to make use of $F(s)$ without creating it.

1083 **3.4 Projected Off-Policy TD (POP-TD)**

1084 We propose an alternative approach to stabilizing off-policy training, based on the
 1085 Non-Expansion Criterion [24]. POP-TD identifies a convex set of “safe” distributions
 1086 that satisfy KNEC and reweights TD updates to come from that set. In contrast to
 1087 TD-DO, POP-TD uses solves a different optimization problem using a two-timescales
 1088 update with fixed cost per iteration, allowing it to scale to real-world problems.

1089 We begin by deriving the projected off-policy update for Markov Chains, without
 1090 a separate policy function. We will extend this derivation to support actions and
 1091 Markov Decision Processes (MDPs) in Section 3.4.5. Our algorithm resamples TD
 1092 updates so they come from some distribution q for which KNEC holds. Given input
 1093 data (x_1, x_2, \dots) , this is the same as finding a set of weights q_1, q_2, \dots such that

$$1094 \quad \sum_i q_i \cdot F(x_i) \succcurlyeq 0 \quad (3.10)$$

1095 3.4.1 I- and M-projections

1096 The Kullback-Leibler divergence is an *asymmetric* measure, and so it is usually
1097 the case that $\min_q \text{KL}(q||\mu) \neq \min_q \text{KL}(\mu||q)$. The former (“from μ to q ”) is
1098 an information (or I-)projection, which tends to under-estimate the support of q
1099 potentially excluding possible sampling distributions to reweigh to. The latter (“from
1100 q to μ ”) is a moment (or M-)projection, which tends to over-estimate the support of
1101 q and avoid zero solutions. In our solution, we are proposing using an I-projection
1102 instead of the M-projection used by Kolter [24].

1103 3.4.2 Optimizing the distribution

1104 In the previous section we have characterized a convex subset of off-policy distributions
1105 under which TD learning is guaranteed not to diverge. If we can discover any such
1106 distribution for a particular TD problem, we can reweigh our TD updates (from any
1107 distribution) so they appear consistent with this reweighing distribution. This is
1108 related to the main insight in Emphatic-TD [49], with the key innovation that we
1109 can take any non-expansive distribution *not just the on-policy distribution*.

1110 We can now write down the optimization problem that we wish to solve:

$$1111 \quad \underset{q}{\text{minimize}} \text{KL}(q||\mu) \quad \text{s.t.} \quad \mathbb{E}_{s \sim q}[F(s)] \succeq 0 \quad (3.11)$$

1112 We are searching for q , the closest distribution to the sampling distribution μ such
1113 that F is PSD under q . Note that we could in principle minimize any notion of
1114 “closest” to find some satisfying distribution – for example Kolter [24] explores the
1115 effects of minimizing $\text{KL}(\mu||q)$.

1116 We construct the dual of this problem:

$$1117 \quad \underset{Z \succ 0}{\text{maximize}} \underset{q}{\text{minimize}} \text{KL}(q||\mu) - \text{tr} Z^\top \mathbb{E}_{s \sim q}[F(s)] \quad (3.12)$$

1118 Using the Lagrange multiplier $Z \in \mathbb{R}^{2k \times 2k}$, we solve the inner optimization problem:

$$1119 \quad \underset{q}{\text{minimize}} \quad -H(q) - \mathbb{E}_{s \sim q}[\log \mu(s) + \text{tr} Z^\top F(s)] \quad (3.13)$$

1120 Writing down Lagrangian and solving for the optima, we obtain:

$$1121 \quad q^*(s) \propto \mu(s) \exp(\text{tr} Z^\top F(s)) \quad (3.14)$$

1122 (Subject to the constraint that $q^*(s)$ is normalized so it must sum to 1 over all s .)

1123 Plugging this back into our dual formulation, we obtain the optimization problem:

$$1124 \quad \underset{Z \succcurlyeq 0}{\text{maximize}} \quad -\log \mathbb{E}_{s \sim \mu}[\exp(\text{tr} Z^\top F(s))] \quad (3.15)$$

1125 Which we can simplify to

$$1126 \quad \underset{Z \succcurlyeq 0}{\text{minimize}} \quad \mathbb{E}_{s \sim \mu}[\exp(\text{tr} Z^\top F(s))] \quad (3.16)$$

1127 As discussed earlier, $F(s)$ cannot be directly constructed; instead, we assume that Z
1128 holds a specific structure and optimize the problem.

1129 **3.4.3 The structure of Z**

1130 Our next goal is to transform this constrained optimization problem into an uncon-
1131 strained problem over a low-rank version of Z , suitable for learning via SGD.

1132 We assume (and later check!) that the solution for Z is low-rank. Intuitively, this is
1133 because $\mathbb{E}_{s \sim \mu}[F(s)]$ is PSD when μ is close to π , and for most MDPs, sampling off-
1134 policy leads to only a small number of negative eigenvalues that need to be corrected
1135 by Z . Kolter [24] provides a technical explanation: by the KKT conditions, Z will
1136 have rank complementary to $\mathbb{E}_{s \sim \mu}[F(s)]$, and the latter is expected to be full rank. It
1137 is worth noting that this “almost-PSD” assumption is common in the field.

1138 We make the strong assumption that Z has rank m , where $m \ll k$. We apply the
 1139 Burer-Montiero approach [4] to convert the constrained optimization problem over Z
 1140 into an unconstrained optimization over matrices $A \in \mathbb{R}^{k \times m}$ and $B \in \mathbb{R}^{k \times m}$:

$$1141 \quad Z^* = \begin{bmatrix} A \\ B \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}^T \quad (3.17)$$

1142 This allows us to represent the rank- m PSD matrix Z^* in terms of the unconstrained
 1143 matrices A and B . Substituting this into the dual formulation, we get:

$$1144 \quad \underset{A, B}{\text{minimize}} \mathbf{E}_{s \sim \mu} \left[\exp \left(\text{tr} \begin{bmatrix} A \\ B \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix}^T F(s) \right) \right] \quad (3.18)$$

1145 We can leverage the structure of $F(s)$ to simplify the trace term:

$$1146 \quad \text{tr} Z^T F(s) \quad (3.19)$$

$$1147 \quad = \text{tr} \begin{bmatrix} A \\ B \end{bmatrix}^T \begin{bmatrix} A \\ B \end{bmatrix} F(s) \quad (3.20)$$

$$1148 \quad = \text{tr} \begin{bmatrix} A \\ B \end{bmatrix}^T F(s) \begin{bmatrix} A \\ B \end{bmatrix} \quad (3.21)$$

$$1149 \quad = \text{tr} \begin{bmatrix} A \\ B \end{bmatrix}^T \mathbf{E}_{s' \sim p(s'|s)} \begin{bmatrix} \phi(s)\phi(s)^T & \phi(s)\phi(s')^T \\ \phi(s')\phi(s)^T & \phi(s)\phi(s)^T \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \quad (3.22)$$

$$1150 \quad = \text{tr} [(A + B)^T \phi(s)\phi(s)^T (A + B) - 2B^T \mathbf{E}_{s' \sim p(s'|s)} [\phi(s)(\phi(s) - \phi(s'))^T] A] \quad (3.23)$$

$$1151 \quad = \|(A + B)^T \phi(s)\|^2 - \text{tr} [2B^T \mathbf{E}_{s' \sim p(s'|s)} [\phi(s)(\phi(s) - \phi(s'))^T] A] \quad (3.24)$$

1152 This allows us to rewrite the optimization problem as:

$$1153 \quad \underset{A, B}{\text{minimize}} \mathbf{E}_{s \sim \mu} \left[\exp \left(\begin{array}{c} \|(A + B)^T \phi(s)\|^2 \\ -\text{tr} [2B^T \mathbf{E}_{s' \sim p(s'|s)} [\phi(s)(\phi(s) - \phi(s'))^T] A] \end{array} \right) \right] \quad (3.25)$$

1154 where the small parameters A and B can be optimized with regular gradient-descent
1155 methods.

1156 3.4.4 Update rules

1157 We can't directly optimize our problem because that would require us to estimate
1158 the inner expectation term. Instead, we use a two-timescales approach by estimating
1159 two (dependent) quantities separately and improving them at potentially different
1160 rates. This (with a little tuning) can generally converge to a valid solution.

1161 We choose to estimate the matrices $A, B \in \mathbb{R}^{k \times m}$ and separately the function $g_\theta : \mathcal{S} \in \mathbb{R}$ where

$$1163 \quad g_\theta(s) \approx \text{tr} Z^T F(s) \quad (3.26)$$

1164 which can be approximated as a linear function (or a neural network) with parameters
1165 θ . The size of the weights learned by POP-TD are therefore $\mathcal{O}(k)$, comparable to the
1166 size of vanilla Q-learning.

1167 This corresponds to the auxiliary loss term for A, B :

$$1168 \quad \mathcal{L}_{A,B}(s, s') = \exp(g_\theta(s)) \left[\|(A + B)^T \phi(s)\|^2 - \text{tr} [2B^T \phi(s)(\phi(s) - \phi(s'))^T A] \right] \quad (3.27)$$

1169 and for g :

$$1170 \quad \mathcal{L}_g(s, s') = (g_\theta(s) - [\|(A + B)^T \phi(s)\|^2 - \text{tr} [2B^T \phi(s)(\phi(s) - \phi(s'))^T A]])^2 \quad (3.28)$$

1171 And finally, to complete this, we multiply each update of w by $\exp(g(s))$ to resample
1172 it so it appears to come from the “safe” distribution, which completes the description
1173 of the algorithm!

1174 **Computing the loss** A naive implementation of the loss function will require
1175 intermediate matrices of size $[k \times k]$. We can improve speed by computing the loss in

1176 terms of $[m \times 1]$ intermediates instead. For some (s, s') , this can be done as:

$$1177 \quad M_A = A^T \phi(s) \in \mathbb{R}^m$$

$$1178 \quad M'_A = A^T \phi(s') \in \mathbb{R}^m$$

$$1179 \quad M_B = B^T \phi(s) \in \mathbb{R}^m$$

$$1180 \quad \mathcal{L}_{A,B}(s, s') \equiv \exp(g_\theta(s)) [\|M_A\|^2 + \|M_B\|^2 + 2M'_A \cdot M_B] \quad (3.29)$$

$$1181 \quad \mathcal{L}_g(s, s') \equiv (g_\theta(s) - [\|M_A\|^2 + \|M_B\|^2 + 2M'_A \cdot M_B])^2 \quad (3.30)$$

1182 where \cdot is the dot product. This sequence of operations should be $\mathcal{O}(mk)$, which is
 1183 much quicker than the naive $\mathcal{O}(mk^2)$.

1184 3.4.5 POP-Q-Learning

1185 Thus far, we have focused on Markov Reward Processes. For RL problems, we need
 1186 to extend this approach to Markov Decision Processes (MDPs). An MDP is a tuple,
 1187 $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$, with state space \mathcal{S} , transition function $P : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow \mathbb{R}_+$, reward
 1188 function $R : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$, and discount factor $\gamma \in [0, 1]$. The goal in this setting is
 1189 to find a probabilistic policy $\pi : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}_+$ that maximizes the future discounted
 1190 reward:

$$1191 \quad \pi^* = \arg \max_{\pi} \mathbb{E}_{\pi} \left[\sum_{t=0}^{\infty} \gamma^t R(s_t, a_t) \right] \quad (3.31)$$

1192 Many RL methods use variations of Q-learning [57, 38, 15, 26], which involves learning
 1193 a state-action value function, or Q-function:

$$1194 \quad Q^{\pi}(s, a) = \mathbb{E}_{\pi} \left[\sum_{t=0}^{\infty} \gamma^t R(s_t, a_t) \mid s_0 = s, a_0 = a \right] \quad (3.32)$$

1195 By considering a fixed policy π , a combined state-space $\mathcal{X} = \mathcal{S} \times \mathcal{A}$, and a policy-
 1196 conditioned transition function $\tilde{P}^{\pi}((s, a), (s', a')) = P(s, a, s')\pi(s', a')$, any MDP
 1197 reduces to a Markov Chain. Thus, as long as the NEC is satisfied in this modified
 1198 state-space, we can bound the approximation error of the Q-function. See Section 3.4.5

Algorithm 1 Deep POP-Q-Learning

Initialize Q-function, Q_{θ^Q} , g-function, g_{θ^g} , dual variable vector y , and some policy π_{θ^π} .

for step t in $1, \dots, N$ **do**

 Sample mini-batch $(s, a, r, s') \sim \mu$.

 Sample $\tilde{a} \sim \pi_{\theta^\pi}(s), \tilde{a}' \sim \pi_{\theta^\pi}(s')$.

 # Compute features from penultimate layer of Q-network:

$\phi \leftarrow Q_{\theta^Q}(s, a), \phi' \leftarrow Q_{\theta^Q}(s', \tilde{a}')$.

 # Update g-function and dual variable vectors:

$\theta_t^g \leftarrow \theta_{t-1}^g - \eta_g \nabla_{\theta^g} \mathcal{L}_g(s, s')$

$A_t \leftarrow A_{t-1} - \eta_A \nabla_A \mathcal{L}_A(s, s')$

$B_t \leftarrow B_{t-1} - \eta_B \nabla_B \mathcal{L}_B(s, s')$

 # Update Q-function using re-weighted Q-loss update:

$\theta_t^Q \leftarrow \theta_{t-1}^Q - \eta_Q \exp(g_{\theta^g}(s, a)) \nabla_{\theta^Q} \mathcal{L}_Q(\theta^Q)$

 # Update policy with SAC-style loss:

$\theta_t^\pi \leftarrow \theta_{t-1}^\pi - \eta_\pi \nabla_{\theta^\pi} [Q_{\theta^Q}(s, \tilde{a}) - \log \pi_{\theta^\pi}(\tilde{a}|s)]$

end for

1199 for a detailed derivation.

1200 Finally, for our method to applied to modern deep RL problems, we must extend our
1201 approach to non-linear Q-functions. To do so, we approximate the Q-function with a
1202 neural network, Q_{θ^Q} parameterized by θ^Q and consider a stochastic parameterized
1203 policy π_{θ^π} . To update Q_{θ^Q} , we used a squared Bellman loss, $\mathcal{L}_Q(\theta^Q) = (Q_{\theta^Q}(s, a) -$
1204 $r - \gamma Q_{\theta^Q}(s', \pi_{\theta^\pi}(s')))^2$, which we reweigh with $e^{g(s)}$ as before. For our offline RL
1205 experiments, we also add CQL regularization [26] to our Q-learning updates to
1206 prevent over-optimism on low-support regions of the state-action space. To update
1207 our linear dual variables y , we use the penultimate layer of Q_{θ^Q} as our feature vector.
1208 Finally, we use a SAC-style entropy regularized loss to update our policy network,
1209 π_{θ^π} . Algorithm 1 provides an overview of our method.

1210 3.5 Experiments and Discussion

1211 We first apply POP-TD to a well-understood example so that we can directly illustrate
1212 the how it resamples TD updates to a “safe” distribution. We use the simple three-
1213 state task from Figure 3.2, including the specified transition function, value function,
1214 and basis. Since this is a policy evaluation task, there is no policy to be separately
1215 learned.

1216 For illustration purposes, we select the family of distributions $\pi = (h/2, h/2, 1 - h)$
1217 parameterized by $h \in [0, 1]$. This characterizes the possible distributions of data
1218 that we will present to POP-TD and naive TD in this experiment. The on-policy
1219 distribution corresponds to $h_o \approx 0.51$, and divides the family of distributions into a
1220 left subset ($h \leq h_o$) where KNEC holds and a right subset ($h_o > 0.5$) where KNEC
1221 does not. This is immediately apparent in Figure 3.2, where we plot the error at
1222 convergence from running naive- and POP-TD above, and the effective distribution of
1223 TD updates after reweighing below. In the left subset, where KNEC holds, POP-TD
1224 does not resample TD updates at all. Therefore, the error of POP-TD tracks naive
1225 TD (top), and the effective distribution of TD updates in POP-TD and naive TD are
1226 the same as the data distribution (bottom).

1227 In the right subset, we observe that naive TD converges to poor solutions with
1228 large error while POP-TD is able to learn with low error. Directly computing the
1229 effective distribution, we see that naive TD adheres to the data distribution but
1230 POP-TD resamples the TD updates. Looking at the behavior of POP-TD in the
1231 right subset, we see that POP-TD resamples updates to the on-policy distribution
1232 p_o in $p \in [p_o, 0.9]$, corresponding to the horizontal segment. This allows the learned
1233 Q-function to have very low error in that domain. As the data distribution becomes
1234 more extreme ($p \in [0.9, 1)$), POP-TD is not quite able to learn the resampling ratio,
1235 and so the effective distribution shifts away from p_o . This leads to a corresponding
1236 slight increase in error at extreme ratios. From this we observe that POP-TD requires
1237 full support of the sampling distribution, similar to many offline RL algorithms [26,
1238 47].

1239 This simple experiment cleanly illustrates how POP-TD resamples TD updates to
1240 come from a “safe” distribution, and how that can greatly reduce the error in a policy
1241 evaluation task.

1242 3.5.1 POP-Q on GridWorld

1243 In this experiment, we consider the the simple grid environment from Figure 3.1,
1244 modified to add transitions from terminating states to the starting state. Our goal
1245 is to approximate the true Q-function with minimal error. Our training data is
1246 sampled following the suboptimal data policy (\dots), adding uniform random dithering
1247 to guarantee that every state-action pair is represented. We represent the Q-function
1248 as a linear function with a fixed random basis $\Phi \in \mathbb{R}^{64 \times 53}$, training it to convergence
1249 using naive Q-learning and linear POP-Q separately. For POP-Q, we also randomly
1250 initialize matrices $A, B \in \mathbb{R}^{53 \times 4}$ and a tabular $g \in \mathbb{R}^{64}$ separately. (We will later
1251 consider an approximate g .)

1252 **Setting the rank of A, B :** We could simply set the rank of A and B as any other
1253 hyperparameter, but since this problem is sufficiently small we can instead compute
1254 the minimum rank directly. To do this, we compute the degree of rank deficiency of
1255 the matrix $\mathbb{E}_s[F(s)]$ from Equation (3.9) on our dataset, and set the rank of A and
1256 B so the sum of the rank of $\mathbb{E}_s[F(s)]$ and A and B is at least k . For this example,
1257 for $k = 53$, we find that $\text{rank}(A) = \text{rank}(B) = 4$ is sufficient for this example.

1258 Results with an exact, tabular g

1259 Since tabular Q-learning always converges to the global optimum [57], we use that to
1260 compute the ground-truth Q-function. All error reported is relative to that assumed
1261 ground truth.

1262 Figure 3.3 shows the distribution of errors achieved by vanilla and POP Q-learning
1263 over 25 different bases on our task. Vanilla Q-learning performs consistently poorly,
1264 achieving a (large) amount of error at all seeds. This is expected because we have
1265 deliberately engineered the task to be unstable. In comparison, POP-TD improves

1266 performance over most seeds, and in some cases enables near-perfect fitting of the
1267 Q-function.

1268 Throughout this chapter we have drawn a distinction between importance sam-
1269 pling/Emphatic TD methods and our work. While the former attempts to resample
1270 to the on-policy distribution, our work seeks to resample to the closest stable distribu-
1271 tion. We illustrate this difference in Figure 3.4, where we display the rates at which
1272 states are visited in our GridWorld. The distribution in our dataset (top-right) is far
1273 from the on-policy distribution (top-left), which is what importance sampling and
1274 Emphatic methods will attempt to resample to. In comparison, POP-Q resamples
1275 minimally (bottom row), where the effective distribution reached is very close to the
1276 data distribution.

1277 **Results with an approximate, linear g**

1278 A key step in adopting POP-Q is ensuring that all parameters are at most order
1279 $\mathcal{O}(k)$ (i.e. comparable to the size of the learned weights) and are therefore learnable
1280 with the same time and space as regular TD. The matrices A and B are sized $k \times m$,
1281 where $m \ll k$, and so are sufficiently small. We now need to approximate g as a
1282 linear function with fixed bases vectors $\Phi_g = (\phi_{g,1}, \phi_{g,2}, \dots, \phi_{g,n})$ and learned weights
1283 $w_g \in \mathbb{R}^l$ of size $l < n$:

$$1284 \quad g(s) = \phi_{g,s} \cdot w_g \quad (3.33)$$

1285 To understand the relationship between the degree of approximation (as measured by
1286 the size of the basis l) and the performance of our system, we initialize 25 different
1287 $n \times n$ bases and report the performance as the bases are truncated down from 64 to
1288 1. This is illustrated in Figure 3.5.

1289 Figure 3.5 reveals that the performance of POP-Q is (as expected) sensitive to the
1290 exact basis chosen. For some bases, the error increases with only a small amount of
1291 approximation, but for some “lottery-ticket” bases, this continues to work even as
1292 the bases are truncated to rank 1. For some bases, this continues to work despite

1293 extreme approximation is because the degree of resampling required is minimal and
1294 the system is fairly easy to resample.

1295 **3.5.2 Linear POP-Q on GridWorld**

1296 The current experiments with POP-Q learning all use a tabular g . This works, but
1297 takes the same memory as would learning a tabular value function, which would
1298 provably converge to the global optimum (side-stepping the entire problem).

1299 Currently, we are evaluating POP-Q with approximate g on our GridWorld example.
1300 We are running an ablation study to understand the relationship between the degree
1301 of approximation of g and the performance of the resultant system.

1302 This is a similar experiment to that in Section 3.5.1, but with linear approximation.
1303 One key step on the road to getting POP-Q to work on larger experiments is
1304 to understand the behavior of POP-Q under function approximation. Function
1305 approximation is necessary because, in the tabular case, POP-Q uses as much
1306 memory as a tabular Q-learning algorithm would; this is intractable for most practical
1307 problems. We also wish to exploit the generalization afforded to us by neural networks,
1308 to hopefully learn more accurate models with less data.

1309 In this experiment, we define $g_\phi : \mathcal{S} \rightarrow \mathbb{R}$ as:

$$1310 \quad g_\phi = \Phi_g \theta^g \quad (3.34)$$

1311 for basis $\Phi_g \in \mathbb{R}^{n \times m}$ and learned weights $\theta^g \in \mathbb{R}^m$. We are given some random Φ_g
1312 and wish to learn θ^g so that g_ϕ acts as the reweighing function of POP-TD.

1313 We conduct a series of experiments to understand the relationship between the degree
1314 of function approximation in g and the quality of the learned model. Our example is
1315 engineered so that the ratio of two specific transitions (where the two trajectories
1316 initially diverge) most determines stability.

1317 When performing experiments, we note that the performance of POP-TD depends
1318 sharply on the condition number of Φ , but not necessarily that of Φ_g . Specifically, we

1319 see that an orthogonal initialization step on Φ is crucial for performance. (In this
1320 step we set Φ to the orthogonal matrix of the QR-decomposition of a matrix where
1321 entries are sampled uniformly at random.) We conjecture that this happens because
1322 POP-TD seeks to stochastically learn $\Phi^T A \Phi$, and a poor condition number of Φ leads
1323 to values that span multiple orders of magnitude and linear approximation is known
1324 to perform poorly on such data.

1325 **3.6 Conclusion**

1326 In this chapter we introduced POP-TD, a method for effective TD learning under
1327 off-policy distributions, with applications to offline RL and learning under large
1328 distribution shifts. Unlike existing emphatic TD and importance sampling methods
1329 which resample to the on-policy distribution, POP-TD resamples to the closest
1330 distribution under which TD will provably not diverge.

1331 We present POP-TD on an existing “deadly triad” example in the literature, showing
1332 how the resampling process operates in theory. We extend this to a more general
1333 GridWorld-style Q-learning task which diverges under vanilla TD, but is consistently
1334 solved by POP-Q-learning.

1335 A key strength of POP-Q-learning is that it achieves all this with a per-loop com-
1336 pute and memory overhead of the same order as Q-learning methods, and can be
1337 implemented and optimized in the same loop as any TD or Q-learning method. In
1338 this sense, it offers a cheap mechanism to stabilize off-policy TD, particularly in the
1339 context of offline RL.

1340 A possible future expansion of this project is to integrate this with an existing
1341 offline RL method such as Conservative Q-Learning (CQL) and examine whether this
1342 improves performance. We propose CQL specifically because it constrains actions
1343 to remain within the support of the data, but does not explicitly constrain the
1344 distribution of states to minimize distribution shift. POP methods require adequate
1345 support (which CQL provides), and in turn are able to minimize distribution shift.

¹³⁴⁶ This suggests that the two algorithms may have some symbiotic relationship.

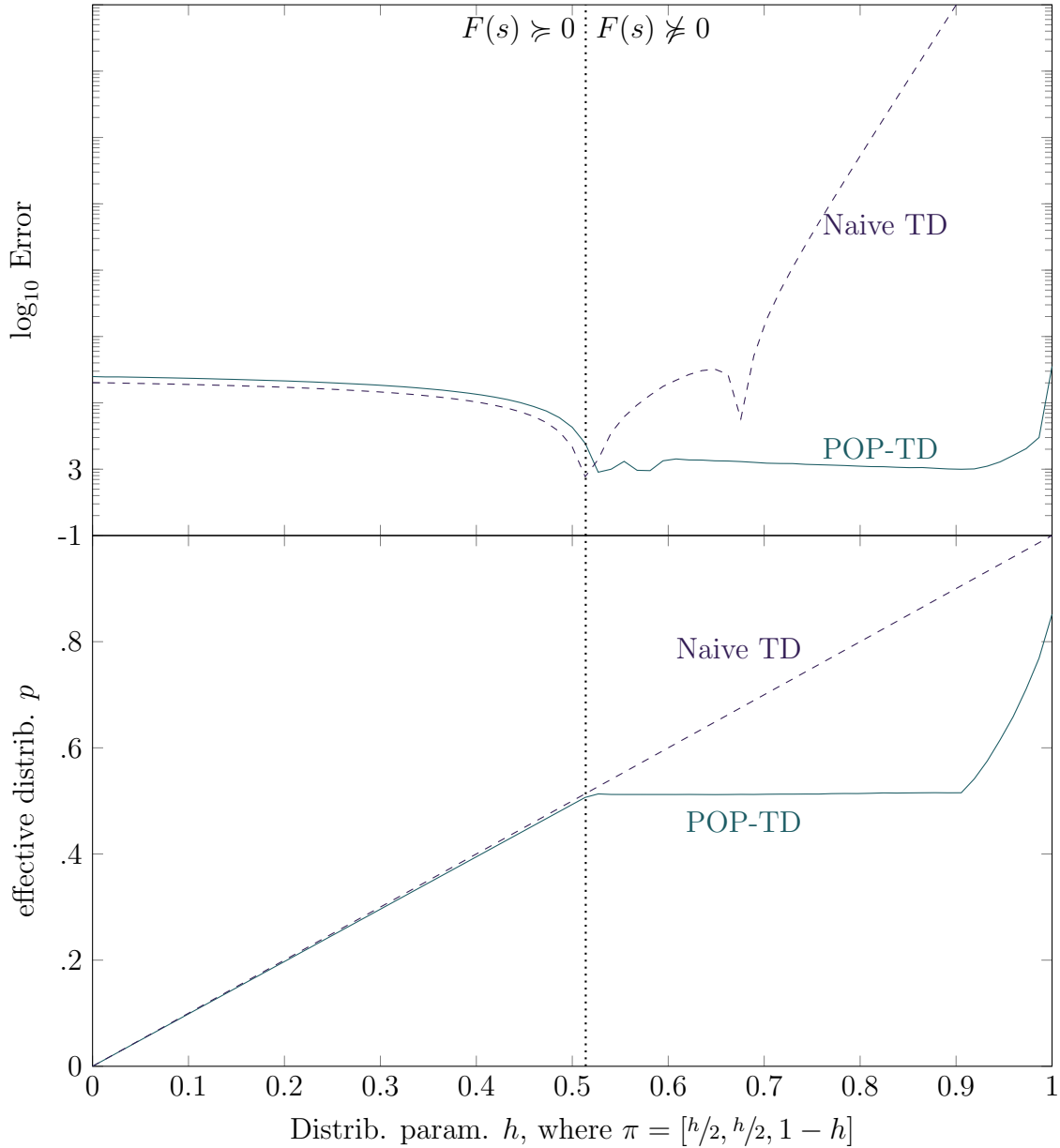


Figure 3.2: The error in the learned value function by naive- and POP-TD, plotted against a varying sampling distribution. In the left half of the plot, KNEC holds, and so POP-TD tracks the error of naive TD closely. In the right half of the plot naive TD diverges, while POP-TD resamples the data to a “safe” distribution and does not diverge.

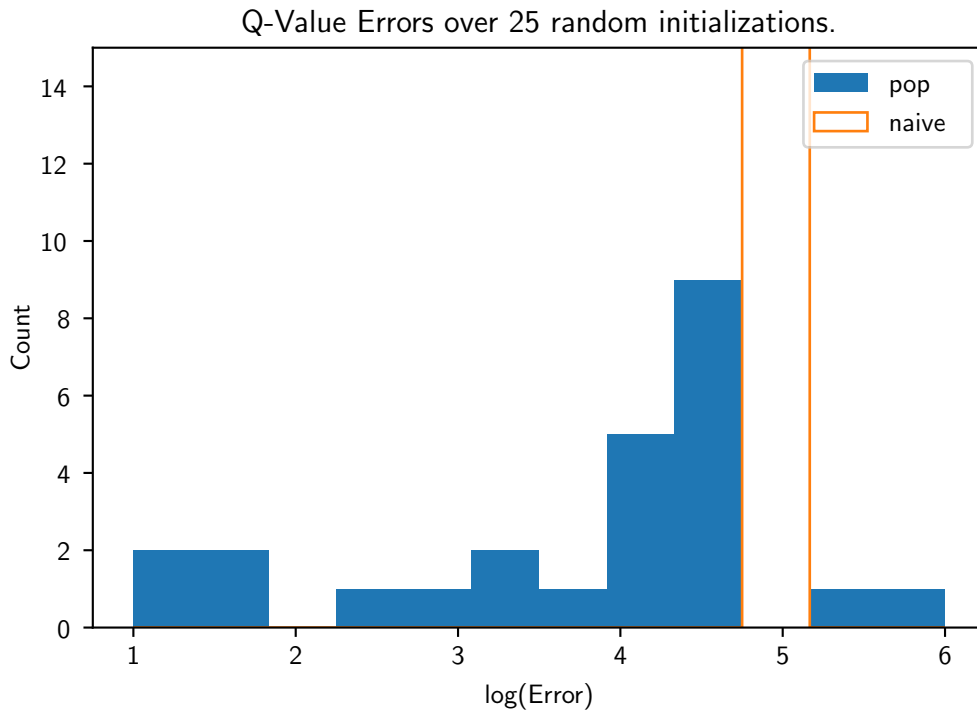


Figure 3.3: Log Q-function errors for naive and POP Q-Learning on Figure 3.1, over 25 randomly sampled bases. Errors are computed using a tabular g function, and bins are exponentially wide. POP-Q substantially reduces error in most of the sampled bases.

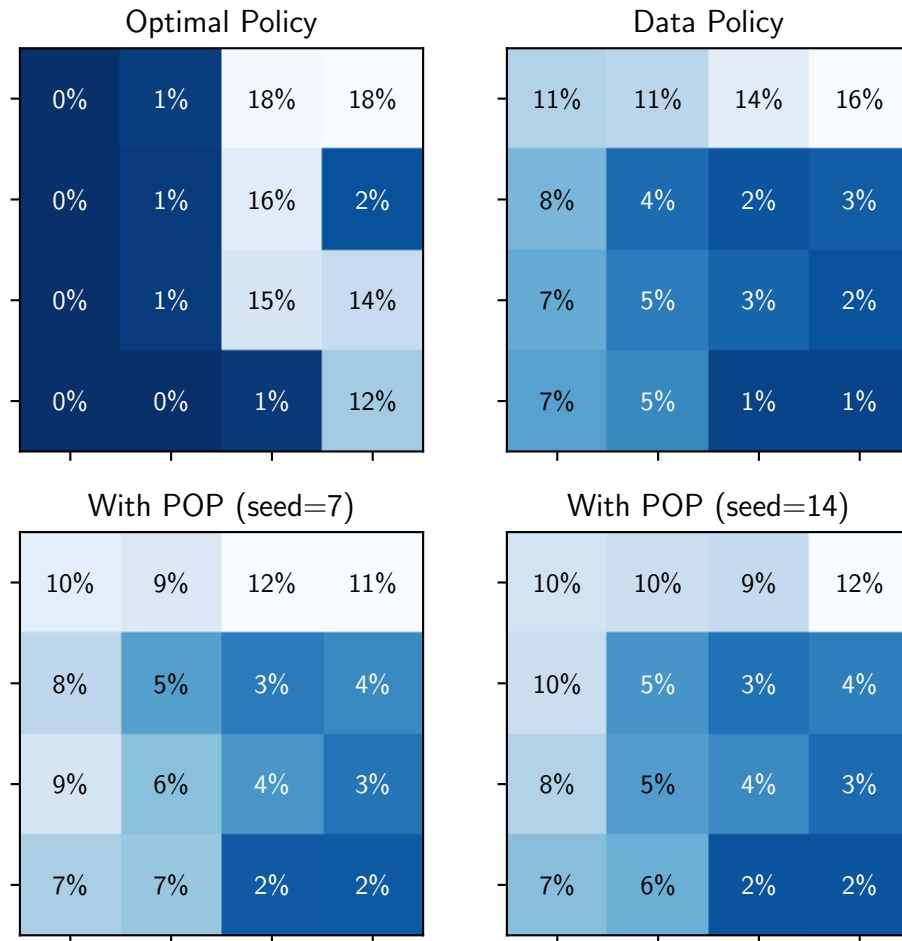


Figure 3.4: Rates at which states are visited in GridWorld. On the top row, we show how the optimal policy (left) is very far from the data policy (right). On the bottom row, we show the effective distribution after POP-Q resamples the data. The effective distribution is very close to the data distribution, despite the tremendous improvement in error.

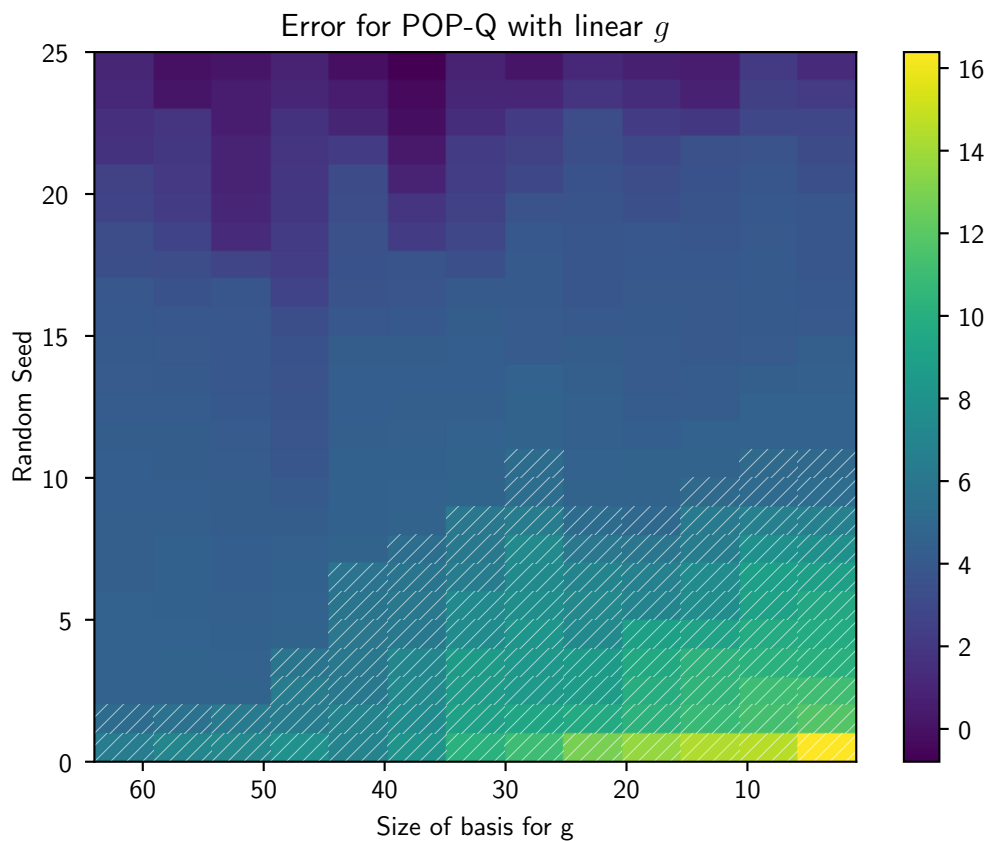


Figure 3.5: Error for POP-Q with linear g functions. Each row corresponds to one starting basis, and each column corresponds to a basis size l as it is reduced from 64 to 1. The hatched cells correspond to combinations of seeds and bases in which POP-Q performs worse than vanilla Q-learning. Under linear approximation POP-Q greatly improves performance over vanilla TD.

Conclusion

1347

1348 We have examined two notions of stability with a subtle relationship: that of learned
1349 dynamics models, and the training of reinforcement learning algorithms. In doing
1350 so, we have introduced new techniques in both areas, as well as filled in a gap in the
1351 literature on the unsuitability of regularization to solve instability in RL.

1352 One key gap in the RL literature that we hope to address in the future is how we
1353 should regularize deep RL in a principled manner. While our prior work shows that
1354 simple ℓ_2 regularization can cause divergence, the literature is ripe for either adaptive
1355 regularization schemes that can detect and avoid pathological behavior, or for novel
1356 non-convex regularization that does not exhibit the same tendency to diverge.

1357 Separately, there remains a large gap in a key area within offline RL in dealing with
1358 the distributional shift problem. While there have been many recent advances in the
1359 field, these advances have been largely incremental, and the field remains ripe for
1360 a novel perspective that can address this. We propose that POP-TD is that novel
1361 perspective. Unlike the existing literature, the key insight that POP-TD brings to
1362 the field is that we can resample to “safe” off-policy distributions that are close to the
1363 data distribution, instead of the on-policy distribution which may be arbitrarily far.
1364 With these novel POP techniques, we hope to allow offline RL to both (1) resample
1365 the data as little as possible thereby preserving the signal in the data, and (2) learn
1366 to generalize from a set of diverse and possibly even adversarial experts that complete
1367 tasks in mutually incompatible ways.

Notation and Definitions

1369 Standard notation for RL concepts through this thesis.

Symbol	Description
$n \in \mathbb{Z}^+$	Number of states.
$k \in \mathbb{Z}^+$	Number of features in the value basis.
$\pi \in \mathbb{R}^n$	on-policy distribution.
$\mu \in \mathbb{R}^n$	sampling distribution, may be on- or off-policy.
$\Phi \in \mathbb{R}^{[n \times k]}$	Feature basis for the value function
$\hat{w} \in \mathbb{R}^{[k \times 1]}$	Linear weights for value function, fit using least-squares regression of V on Φ .
$w^*(\eta) \in \mathbb{R}^{[k \times 1]}$	Linear weights for value function, learned using TD.
$\Phi w^*(\eta) \in \mathbb{R}^{[n \times 1]}$	Learned value function
$V \in \mathbb{R}^{[n \times 1]}$	True value function
$\ V\ \in \mathbb{R}$	Error from guessing zeros, equivalent to the threshold for a vacuous example
$\ x\ \in \mathbb{R}_0^+$	ℓ_2 -norm of vector or matrix x , equal to $\sqrt{x^\top x}$
$\ x\ _D \in \mathbb{R}_0^+$	ℓ_2 -norm of vector or matrix x under D , equal to $\sqrt{x^\top D x}$

1370 **Regularization**

Symbol	Description
$\eta \in \mathbb{R}_0^+$	ℓ_2 regularization parameter
$h \in [0, 1]$	distribution parameter used to express a family of possible sampling distributions.
$\eta_m \in \mathbb{R}_0^+$	ℓ_2 regularization parameter for emphasis model in COF-PAC (the Emphatic algorithm we analyze)
$\eta_v \in \mathbb{R}_0^+$	ℓ_2 regularization parameter for value model in COF-PAC (the Emphatic algorithm we analyze)
$v : \mathbb{R}^+ \rightarrow \mathbb{R}^n$	apparent distribution induced by η -regularizing the emphatic correction of off-policy μ to on-policy π

1371 **Projected Off-Policy**

Symbol	Description
$m \in \mathbb{Z}^+$	Number of features in the g -basis (for POP methods).
$l \in \mathbb{Z}^+$	Rank of A and B two-timescales parameters (for POP methods).
$g : \mathcal{S} \rightarrow \mathbb{R}$	dual objective component, learned opposite A and B in POP methods.
$e^{g(s)} \in \mathbb{R}^+$	The resampling coefficient for TD updates from state s
$\Phi_g \in \mathbb{R}^{[n \times m]}$	Feature basis for the learned linear g function
$w_g \in \mathbb{R}^{[m \times 1]}$	Linear weights for learned g function
$A, B \in \mathbb{R}^{[k \times l]}$	Two-timescales parameters learned alongside g in POP methods, where $l \ll k$.
$\Phi_g w_g \in \mathbb{R}^{[n \times 1]}$	Learned g function

Bibliography

- [1] Brandon Amos, Lei Xu, and J Zico Kolter. “Input convex neural networks”. In: *Proceedings of the 34th International Conference on Machine Learning-Volume 70*. JMLR.org. 2017, pp. 146–155.
- [2] Caroline Blocher, Matteo Saveriano, and Dongheui Lee. “Learning stable dynamical systems using contraction theory”. In: *2017 14th International Conference on Ubiquitous Robots and Ambient Intelligence (URAI)*. IEEE. 2017, pp. 124–129.
- [3] Byron Boots, Geoffrey J Gordon, and Sajid M Siddiqi. “A constraint generation approach to learning stable linear dynamical systems”. In: *Advances in neural information processing systems*. 2008, pp. 1329–1336.
- [4] Samuel Burer and Renato DC Monteiro. “A nonlinear programming algorithm for solving semidefinite programs via low-rank factorization”. In: *Mathematical Programming* 95.2 (2003), pp. 329–357.
- [5] Yize Chen, Yuanyuan Shi, and Baosen Zhang. “Optimal Control Via Neural Networks: A Convex Approach”. In: *arXiv preprint arXiv:1805.11835* (2018).
- [6] Yinlam Chow et al. “A Lyapunov-based approach to safe reinforcement learning”. In: *Advances in Neural Information Processing Systems*. 2018, pp. 8092–8101.
- [7] Jonas Degraeve et al. “Magnetic control of tokamak plasmas through deep reinforcement learning”. In: *Nature* 602.7897 (2022), pp. 414–419.
- [8] Raghuram Bharadwaj Diddigi, Chandramouli Kamanchi, and Shalabh Bhatnagar. “A convergent off-policy temporal difference algorithm”. In: *arXiv preprint arXiv:1911.05697* (2019).

- 1395 [9] Simon S Du et al. “Stochastic variance reduction methods for policy evaluation”.
1396 In: *International Conference on Machine Learning*. PMLR. 2017, pp. 1049–1058.
- 1397 [10] William Fedus et al. “Revisiting fundamentals of experience replay”. In: *Inter-*
1398 *national Conference on Machine Learning*. PMLR. 2020, pp. 3061–3071.
- 1399 [11] Scott Fujimoto, David Meger, and Doina Precup. “Off-policy deep reinforcement
1400 learning without exploration”. In: *International conference on machine learning*.
1401 PMLR. 2019, pp. 2052–2062.
- 1402 [12] Yarin Gal, Rowan McAllister, and Carl Edward Rasmussen. “Improving PILCO
1403 with Bayesian neural network dynamics models”. In: *Data-Efficient Machine*
1404 *Learning workshop, ICML*. Vol. 4. 2016.
- 1405 [13] Carles Gelada and Marc G Bellemare. “Off-policy deep reinforcement learning
1406 by bootstrapping the covariate shift”. In: *Proceedings of the AAAI Conference*
1407 *on Artificial Intelligence*. Vol. 33. 01. 2019, pp. 3647–3655.
- 1408 [14] Shixiang Gu et al. “Continuous deep q-learning with model-based acceleration”.
1409 In: *International Conference on Machine Learning*. 2016, pp. 2829–2838.
- 1410 [15] Tuomas Haarnoja et al. “Soft actor-critic: Off-policy maximum entropy deep
1411 reinforcement learning with a stochastic actor”. In: *International conference on*
1412 *machine learning*. PMLR. 2018, pp. 1861–1870.
- 1413 [16] Assaf Hallak and Shie Mannor. “Consistent on-line off-policy evaluation”. In:
1414 *International Conference on Machine Learning*. PMLR. 2017, pp. 1372–1383.
- 1415 [17] Hado van Hasselt et al. “Expected eligibility traces”. In: *arXiv preprint arXiv:2007.01839*
1416 (2021).
- 1417 [18] Kaiming He et al. “Delving deep into rectifiers: Surpassing human-level perfor-
1418 mance on imagenet classification”. In: *Proceedings of the IEEE international*
1419 *conference on computer vision*. 2015, pp. 1026–1034.
- 1420 [19] Ray Jiang et al. “Learning Expected Emphatic Traces for Deep RL”. In: *arXiv*
1421 *preprint arXiv:2107.05405* (2021).
- 1422 [20] Hassan K Khalil and Jessy W Grizzle. *Nonlinear systems*. Vol. 3. Prentice hall
1423 Upper Saddle River, NJ, 2002.

- 1424 [21] S Mohammad Khansari-Zadeh and Aude Billard. “Learning stable nonlinear
1425 dynamical systems with gaussian mixture models”. In: *IEEE Transactions on*
1426 *Robotics* 27.5 (2011), pp. 943–957.
- 1427 [22] Rahul Kidambi et al. “Morel: Model-based offline reinforcement learning”. In:
1428 *Advances in neural information processing systems* 33 (2020), pp. 21810–21823.
- 1429 [23] Diederik P Kingma and Max Welling. “Auto-encoding variational bayes”. In:
1430 *arXiv preprint arXiv:1312.6114* (2013).
- 1431 [24] J Kolter. “The fixed points of off-policy TD”. In: *Advances in Neural Information*
1432 *Processing Systems* 24 (2011), pp. 2169–2177.
- 1433 [25] Aviral Kumar, Abhishek Gupta, and Sergey Levine. “Discor: Corrective feed-
1434 back in reinforcement learning via distribution correction”. In: *arXiv preprint*
1435 *arXiv:2003.07305* (2020).
- 1436 [26] Aviral Kumar et al. “Conservative Q-Learning for Offline Reinforcement Learn-
1437 ing”. In: *Advances in Neural Information Processing Systems 33: Annual Con-*
1438 *ference on Neural Information Processing Systems 2020, NeurIPS 2020, De-*
1439 *cember 6-12, 2020, virtual*. Ed. by Hugo Larochelle et al. 2020. URL: [https://](https://proceedings.neurips.cc/paper/2020/hash/0d2b2061826a5df3221116a5085a6052-Abstract.html)
1440 [proceedings.neurips.cc/paper/2020/hash/0d2b2061826a5df3221116a5085a6052-](https://proceedings.neurips.cc/paper/2020/hash/0d2b2061826a5df3221116a5085a6052-Abstract.html)
1441 [Abstract.html](https://proceedings.neurips.cc/paper/2020/hash/0d2b2061826a5df3221116a5085a6052-Abstract.html).
- 1442 [27] Aviral Kumar et al. “DR3: Value-Based Deep Reinforcement Learning Requires
1443 Explicit Regularization”. In: *International Conference on Learning Representa-*
1444 *tions*. 2022. URL: <https://openreview.net/forum?id=P0vMvLi91f>.
- 1445 [28] Aviral Kumar et al. “Stabilizing off-policy q-learning via bootstrapping error
1446 reduction”. In: *Advances in Neural Information Processing Systems* 32 (2019).
- 1447 [29] Joseph La Salle and Solomon Lefschetz. *Stability by Liapunov’s Direct Method*
1448 *with Applications by Joseph L Salle and Solomon Lefschetz*. Vol. 4. Elsevier,
1449 2012.
- 1450 [30] Sergey Levine et al. “Offline Reinforcement Learning: Tutorial, Review, and
1451 Perspectives on Open Problems”. In: *CoRR* abs/2005.01643 (2020). arXiv:
1452 2005.01643. URL: <https://arxiv.org/abs/2005.01643>.

- 1453 [31] Sergey Levine et al. “Offline Reinforcement Learning: Tutorial, Review, and
1454 Perspectives on Open Problems”. In: *CoRR* abs/2005.01643 (2020). arXiv:
1455 2005.01643. URL: <https://arxiv.org/abs/2005.01643>.
- 1456 [32] Qiang Liu et al. “Breaking the curse of horizon: Infinite-horizon off-policy
1457 estimation”. In: *Advances in Neural Information Processing Systems* 31 (2018).
- 1458 [33] Sridhar Mahadevan et al. “Proximal reinforcement learning: A new theory of se-
1459 quential decision making in primal-dual spaces”. In: *arXiv preprint arXiv:1405.6757*
1460 (2014).
- 1461 [34] Gaurav Manek and J Zico Kolter. “Learning stable deep dynamics models”. In:
1462 *Advances in neural information processing systems* 32 (2019).
- 1463 [35] Gaurav Manek and J Zico Kolter. “The Pitfalls of Regularization in Off-Policy
1464 TD Learning”. In: *Advances in Neural Information Processing Systems*. Ed.
1465 by Alice H. Oh et al. 2022. URL: <https://openreview.net/forum?id=vK53GLZJes8>.
- 1467 [36] Gaurav Manek, Melrose Roderick, and J Zico Kolter. “Projected Off-Policy TD
1468 Learning Stabilize Offline Reinforcement Learning”. In: Jan. 2023.
- 1469 [37] Nikhil Mishra, Pieter Abbeel, and Igor Mordatch. “Prediction and control with
1470 temporal segment models”. In: *Proceedings of the 34th International Conference*
1471 *on Machine Learning-Volume 70*. JMLR. org. 2017, pp. 2459–2468.
- 1472 [38] Volodymyr Mnih et al. “Human-level control through deep reinforcement learn-
1473 ing”. In: *Nature* 518.7540 (Feb. 2015), pp. 529–533. ISSN: 00280836. URL: <http://dx.doi.org/10.1038/nature14236>.
- 1475 [39] Ofir Nachum et al. “Algaedice: Policy gradient from arbitrary experience”. In:
1476 *arXiv preprint arXiv:1912.02074* (2019).
- 1477 [40] Ofir Nachum et al. “Dualdice: Behavior-agnostic estimation of discounted sta-
1478 tionary distribution corrections”. In: *Advances in Neural Information Processing*
1479 *Systems* 32 (2019).
- 1480 [41] Anusha Nagabandi et al. “Neural network dynamics for model-based deep
1481 reinforcement learning with model-free fine-tuning”. In: *2018 IEEE International*
1482 *Conference on Robotics and Automation (ICRA)*. IEEE. 2018, pp. 7559–7566.

- 1483 [42] Antonis Papachristodoulou and Stephen Prajna. “On the construction of Lyapunov functions using the sum of squares decomposition”. In: *Proceedings of the 41st IEEE Conference on Decision and Control, 2002*. Vol. 3. IEEE. 2002, pp. 3482–3487.
- 1484
1485
1486
- 1487 [43] Pablo A Parrilo. “Structured semidefinite programs and semialgebraic geometry methods in robustness and optimization”. PhD thesis. California Institute of Technology, 2000.
- 1488
1489
- 1490 [44] Doina Precup. “Eligibility traces for off-policy policy evaluation”. In: *Computer Science Department Faculty Publication Series* (2000), p. 80.
- 1491
- 1492 [45] Spencer M Richards, Felix Berkenkamp, and Andreas Krause. “The Lyapunov neural network: Adaptive stability certification for safe learning of dynamic systems”. In: *arXiv preprint arXiv:1808.00924* (2018).
- 1493
1494
- 1495 [46] Arno Schödl et al. “Video textures”. In: *Proceedings of the 27th annual conference on Computer graphics and interactive techniques*. ACM Press/Addison-Wesley Publishing Co. 2000, pp. 489–498.
- 1496
1497
- 1498 [47] Laixi Shi et al. “Pessimistic q-learning for offline reinforcement learning: Towards optimal sample complexity”. In: *arXiv preprint arXiv:2202.13890* (2022).
- 1499
- 1500 [48] Richard S Sutton and Andrew G Barto. *Reinforcement learning: An introduction*. Second Edition. MIT press, 2020.
- 1501
- 1502 [49] Richard S Sutton, A Rupam Mahmood, and Martha White. “An emphatic approach to the problem of off-policy temporal-difference learning”. In: *The Journal of Machine Learning Research* 17 (2016), pp. 2603–2631.
- 1503
1504
- 1505 [50] Richard S Sutton et al. “Fast gradient-descent methods for temporal-difference learning with linear function approximation”. In: *Proceedings of the 26th Annual International Conference on Machine Learning*. 2009, pp. 993–1000.
- 1506
1507
- 1508 [51] Andrew J Taylor et al. “Episodic Learning with Control Lyapunov Functions for Uncertain Robotic Systems”. In: *arXiv preprint arXiv:1903.01577* (2019).
- 1509
- 1510 [52] Andrey Nikolayevich Tikhonov. “On the stability of inverse problems”. In: *Dokl. Akad. Nauk SSSR*. Vol. 39. 1943, pp. 195–198.
- 1511

- 1512 [53] JN Tsitsiklis and B Van Roy. “An analysis of temporal-difference learning
1513 with function approximation”. In: *Rep. LIDS-P-2322). Lab. Inf. Decis. Syst.*
1514 *Massachusetts Inst. Technol. Tech. Rep* (1996).
- 1515 [54] Jonas Umlauft and Sandra Hirche. “Learning stable stochastic nonlinear dynam-
1516 ical systems”. In: *Proceedings of the 34th International Conference on Machine*
1517 *Learning-Volume 70*. JMLR. org. 2017, pp. 3502–3510.
- 1518 [55] Jake VanderPlas. *Triple Pendulum CHAOS!* [http://jakevdp.github.io/
1519 blog/2017/03/08/triple-pendulum-chaos/](http://jakevdp.github.io/blog/2017/03/08/triple-pendulum-chaos/). Mar. 2017.
- 1520 [56] Andrew J Wagenmaker et al. “First-Order Regret in Reinforcement Learning
1521 with Linear Function Approximation: A Robust Estimation Approach”. In:
1522 *Proceedings of the 39th International Conference on Machine Learning*. Ed. by
1523 Kamalika Chaudhuri et al. Vol. 162. Proceedings of Machine Learning Research.
1524 PMLR, July 2022, pp. 22384–22429. URL: [https://proceedings.mlr.press/
1525 v162/wagenmaker22a.html](https://proceedings.mlr.press/v162/wagenmaker22a.html).
- 1526 [57] Christopher JCH Watkins and Peter Dayan. “Q-learning”. In: *Machine learning*
1527 8.3 (1992), pp. 279–292.
- 1528 [58] Ronald J Williams and Leemon C Baird III. *Analysis of some incremental*
1529 *variants of policy iteration: First steps toward understanding actor-critic learning*
1530 *systems*. Tech. rep. Citeseer, 1993.
- 1531 [59] Yifan Wu, George Tucker, and Ofir Nachum. “Behavior regularized offline
1532 reinforcement learning”. In: *arXiv preprint arXiv:1911.11361* (2019).
- 1533 [60] Huizhen Yu. “On convergence of some gradient-based temporal-differences
1534 algorithms for off-policy learning”. In: *arXiv preprint arXiv:1712.09652* (2017).
- 1535 [61] Tianhe Yu et al. “Mopo: Model-based offline policy optimization”. In: *Advances*
1536 *in Neural Information Processing Systems* 33 (2020), pp. 14129–14142.
- 1537 [62] Shangdong Zhang, Hengshuai Yao, and Shimon Whiteson. “Breaking the Deadly
1538 Triad with a Target Network”. In: *CoRR* abs/2101.08862 (2021). arXiv: 2101.
1539 08862. URL: <https://arxiv.org/abs/2101.08862>.

- 1540 [63] Shangtong Zhang et al. “Provably convergent two-timescale off-policy actor-
1541 critic with function approximation”. In: *International Conference on Machine*
1542 *Learning*. PMLR. 2020, pp. 11204–11213.