Analyses of Policy Gradient for Language Model Finetuning and Optimal Control

Noam Razin Tel Aviv University

MML Seminar MPI MIS + UCLA 7 March 2024









Gradient-based methods are the workhorse behind optimization and generalization in modern machine learning

Supervised Learning



Task: Learn predictor minimizing loss over labeled data

Training Algorithm: Gradient descent

Supervised Learning



Task: Learn predictor minimizing loss over labeled data

Training Algorithm: Gradient descent

Optimization Dynamics and Implicit Bias



(e.g., Neyshabur et al. 2014, Gunasekar et al. 2017, Soudry et al. 2018, Arora et al. 2019, Ji & Telgarsky 2019; **R** et al. 2020/21/22, Pesme et al. 2021, Lyu et al. 2021, Boursier et al. 2022, Andriushchenko et al. 2023, Frei et al. 2023, Jin & Montúfar 2023, Abbe et al. 2023)

Supervised Learning



Task: Learn predictor minimizing loss over labeled data

Training Algorithm: Gradient descent

Optimization Dynamics and Implicit Bias



(e.g., Neyshabur et al. 2014, Gunasekar et al. 2017, Soudry et al. 2018, Arora et al. 2019, Ji & Telgarsky 2019; **R** et al. 2020/21/22, Pesme et al. 2021, Lyu et al. 2021, Boursier et al. 2022, Andriushchenko et al. 2023, Frei et al. 2023, Jin & Montúfar 2023, Abbe et al. 2023)

Optimal Control/Reinforcement Learning



Task: Learn policy minimizing cost/maximizing reward over **dynamical system**

Training Algorithm: Policy gradient

Supervised Learning



Task: Learn predictor minimizing loss over labeled data

Training Algorithm: Gradient descent

Optimization Dynamics and Implicit Bias



(e.g., Neyshabur et al. 2014, Gunasekar et al. 2017, Soudry et al. 2018, Arora et al. 2019, Ji & Telgarsky 2019; **R** et al. 2020/21/22, Pesme et al. 2021, Lyu et al. 2021, Boursier et al. 2022, Andriushchenko et al. 2023, Frei et al. 2023, Jin & Montúfar 2023, Abbe et al. 2023)

Optimal Control/Reinforcement Learning



Task: Learn policy minimizing cost/maximizing reward over **dynamical system**

Training Algorithm: Policy gradient

Optimization Dynamics and Implicit Bias

ed Understan

(Fazel et al. 2018, Mei et al. 2020, Hu et al. 2021)

Sources

Optimization

Vanishing Gradients in Reinforcement Finetuning of Language Models

Ú

R + Zhou + Saremi + Thilak + Bradley + Nakkiran + Susskind + Littwin | *ICLR* 2024

Implicit Bias

Implicit Bias of Policy Gradient in Linear Quadratic Control: Extrapolation to Unseen Initial States

R + Alexander + Cohen-Karlik + Giryes + Globerson + Cohen | *arXiv* 2024

Vanishing Gradients in Reinforcement Finetuning of Language Models

R + Zhou + Saremi + Thilak + Bradley + Nakkiran + Susskind + Littwin | *ICLR* 2024



Language Model (LM): Neural network trained on large amounts of text data to produce a **distribution over text**



Language Model (LM): Neural network trained on large amounts of text data to produce a **distribution over text**



Language Model (LM): Neural network trained on large amounts of text data to produce a **distribution over text**



LMs are typically autoregressive

Language Model (LM): Neural network trained on large amounts of text data to produce a **distribution over text**



LMs are typically autoregressive $p_{\theta}(\mathbf{y}|\mathbf{x}) = \prod_{l=1}^{L} p_{\theta}(\mathbf{y}_{l}|\mathbf{x}, \mathbf{y}_{\leq l-1})$

Language Model (LM): Neural network trained on large amounts of text data to produce a **distribution over text**



LMs are typically autoregressive $p_{\theta}(\mathbf{y}|\mathbf{x}) = \prod_{l=1}^{L} p_{\theta}(\mathbf{y}_{l}|\mathbf{x}, \mathbf{y}_{\leq l-1})$

softmax is used for producing next-token probabilities

LMs are adapted to human preferences and downstream tasks via finetuning

LMs are adapted to human preferences and downstream tasks via finetuning

Supervised Finetuning (SFT)

Minimize cross entropy loss over labeled inputs via gradient-based methods



LMs are adapted to human preferences and downstream tasks via finetuning

Supervised Finetuning (SFT)

Minimize cross entropy loss over labeled inputs via gradient-based methods





LMs are adapted to human preferences and downstream tasks via finetuning

Supervised Finetuning (SFT)

Minimize cross entropy loss over labeled inputs via gradient-based methods



Limitations:

Hard to formalize human preferences through labels

LMs are adapted to human preferences and downstream tasks via **finetuning**

Supervised Finetuning (SFT)

Minimize cross entropy loss over labeled inputs via gradient-based methods



Limitations:



Hard to formalize human preferences through labels

S) Labeled data is expensive

Limitations of SFT led to wide adoption of a reinforcement learning-based approach

(e.g. Ziegler et al. 2019, Stiennon et al. 2020, Ouyang et al. 2022, Bai et al. 2022, Dubois et al. 2023, Touvron et al. 2023)

Limitations of SFT led to wide adoption of a reinforcement learning-based approach

(e.g. Ziegler et al. 2019, Stiennon et al. 2020, Ouyang et al. 2022, Bai et al. 2022, Dubois et al. 2023, Touvron et al. 2023)

Reinforcement Finetuning (RFT)

Maximize reward over unlabeled inputs via **policy gradient algorithms**



Limitations of SFT led to wide adoption of a reinforcement learning-based approach

(e.g. Ziegler et al. 2019, Stiennon et al. 2020, Ouyang et al. 2022, Bai et al. 2022, Dubois et al. 2023, Touvron et al. 2023)

Reinforcement Finetuning (RFT)

Maximize reward over unlabeled inputs via **policy gradient algorithms**

equal to a set of the set of th

Expected reward for input x: $V_{\theta}(\mathbf{x}) = \mathbb{E}_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]$

Limitations of SFT led to wide adoption of a reinforcement learning-based approach

(e.g. Ziegler et al. 2019, Stiennon et al. 2020, Ouyang et al. 2022, Bai et al. 2022, Dubois et al. 2023, Touvron et al. 2023)

Reinforcement Finetuning (RFT)

Maximize reward over unlabeled inputs via **policy gradient algorithms**

Figure, **•••**, **Figure** reward function $r(\mathbf{x}, \mathbf{y})$

Expected reward for input x: $V_{\theta}(\mathbf{x}) = \mathbb{E}_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]$

Reward function $r(\mathbf{x}, \mathbf{y})$ can be:

Limitations of SFT led to wide adoption of a reinforcement learning-based approach

(e.g. Ziegler et al. 2019, Stiennon et al. 2020, Ouyang et al. 2022, Bai et al. 2022, Dubois et al. 2023, Touvron et al. 2023)

Reinforcement Finetuning (RFT)

Maximize reward over unlabeled inputs via **policy gradient algorithms**

Expected reward for input x: $V_{\theta}(\mathbf{x}) = \mathbb{E}_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]$

Reward function $r(\mathbf{x}, \mathbf{y})$ can be:



Limitations of SFT led to wide adoption of a reinforcement learning-based approach

(e.g. Ziegler et al. 2019, Stiennon et al. 2020, Ouyang et al. 2022, Bai et al. 2022, Dubois et al. 2023, Touvron et al. 2023)

Reinforcement Finetuning (RFT)

Maximize reward over unlabeled inputs via **policy gradient algorithms**

—, **—**, ••• reward function $r(\mathbf{x}, \mathbf{y})$

Expected reward for input **x**: $V_{\theta}(\mathbf{x}) = \mathbb{E}_{\mathbf{v} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]$

Reward function $r(\mathbf{x}, \mathbf{y})$ can be:



Learned from human preferences







Fundamental vanishing gradients problem in RFT



Vanishing gradients are prevalent and harm ability to maximize reward



problem in RFT



Vanishing gradients are prevalent and harm ability to maximize reward



Exploring ways to overcome vanishing gradients in RFT





Vanishing gradients are prevalent and harm ability to maximize reward



Exploring ways to overcome vanishing gradients in RFT

Vanishing Gradients Due to Small Reward Standard Deviation (STD)

 $STD_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})}[r(\mathbf{x}, \mathbf{y})]$ – reward std of \mathbf{x} under the model
$STD_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})}[r(\mathbf{x}, \mathbf{y})]$ – reward std of \mathbf{x} under the model

Theorem

$$\|\nabla_{\theta} V_{\theta}(\mathbf{x})\| = O\left(\mathrm{STD}_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]^{2/3}\right)$$

*Same holds for PPO gradient

 $STD_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})}[r(\mathbf{x}, \mathbf{y})]$ – reward std of \mathbf{x} under the model

Theorem

$$\|\nabla_{\theta} V_{\theta}(\mathbf{x})\| = O\left(\mathrm{STD}_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]^{2/3}\right)$$

*Same holds for PPO gradient

 Expected gradient for an input vanishes when reward std is small, even if reward mean is suboptimal

 $STD_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})}[r(\mathbf{x}, \mathbf{y})]$ – reward std of \mathbf{x} under the model

Theorem

$$\|\nabla_{\theta} V_{\theta}(\mathbf{x})\| = O\left(\mathrm{STD}_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]^{2/3}\right)$$

*Same holds for PPO gradient

 Expected gradient for an input vanishes when reward std is small, even if reward mean is suboptimal

Proof Idea: Stems from use of softmax + reward maximization objective

 $STD_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})}[r(\mathbf{x}, \mathbf{y})]$ – reward std of \mathbf{x} under the model

Theorem

$$\|\nabla_{\theta} V_{\theta}(\mathbf{x})\| = O\left(\mathrm{STD}_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]^{2/3}\right)$$

*Same holds for PPO gradient

 Expected gradient for an input vanishes when reward std is small, even if reward mean is suboptimal

Proof Idea: Stems from use of softmax + reward maximization objective

Note: Bound applies to expected gradients of individual inputs (as opposed to of batch/population)

 $STD_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})}[r(\mathbf{x}, \mathbf{y})]$ – reward std of \mathbf{x} under the model

Theorem

$$\|\nabla_{\theta} V_{\theta}(\mathbf{x})\| = O\left(\mathrm{STD}_{\mathbf{y} \sim p_{\theta}(\cdot | \mathbf{x})} [r(\mathbf{x}, \mathbf{y})]^{2/3}\right)$$

*Same holds for PPO gradient

 Expected gradient for an input vanishes when reward std is small, even if reward mean is suboptimal

Proof Idea: Stems from use of softmax + reward maximization objective

Note: Bound applies to expected gradients of individual inputs (as opposed to of batch/population)

Can be problematic when finetuning text distribution differs from pretraining

Main Contributions: Vanishing Gradients in RFT



 $abla heta \mathbf{V}_{\theta}(\mathbf{x}) \approx \mathbf{0}$ Fundamental vanishing gradients
problem in DEE problem in RFT



Vanishing gradients are prevalent and harm ability to maximize reward



Exploring ways to overcome vanishing gradients in RFT

Benchmark: GRUE (Ramamurthy et al. 2023) 7 language generation datasets

<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>M</u> 7 language generation datasets

Models: GPT-2 and T5-base

<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Models</u>: GPT-2 and T5-base 7 language generation datasets

Finding I

3 of 7 datasets contain considerable # of train inputs with small reward std and low reward

Benchmark: GRUE (Ramamurthy et al. 2023) Models: GPT-2 and T5-base 7 language generation datasets



<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) 7 language generation datasets

Models: GPT-2 and T5-base

vanishing gradients



3 of 7 datasets contain considerable # of train inputs with small reward std and low reward





<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Models</u>: GPT-2 and T5-base 7 language generation datasets

Finding I

3 of 7 datasets contain considerable # of train inputs with small reward std and low reward

NarrativeQA (many inputs w/ small std)



vanishing gradients



<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>M</u> 7 language generation datasets

Models: GPT-2 and T5-base

<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Models</u>: GPT-2 and T5-base 7 language generation datasets

Finding II

12/38

<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Models</u>: GPT-2 and T5-base 7 language generation datasets

Finding II



<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Models</u>: GPT-2 and T5-base 7 language generation datasets

Finding II



<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Models</u>: GPT-2 and T5-base 7 language generation datasets

Finding II



<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Mo</u> 7 language generation datasets

Models: GPT-2 and T5-base

Finding III

<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Models</u>: GPT-2 and T5-base 7 language generation datasets

Finding III

RFT performance is worse when inputs with small reward std are prevalent

<u>Benchmark</u>: GRUE (Ramamurthy et al. 2023) <u>Models</u>: GPT-2 and T5-base 7 language generation datasets

Finding III

RFT performance is worse when inputs with small reward std are prevalent



Main Contributions: Vanishing Gradients in RFT



 $\nabla_{\theta} \mathbf{V}_{\theta}(\mathbf{x}) \approx \mathbf{0}$ Fundamental vanishing gradients problem in RFT



Vanishing gradients are prevalent and harm ability to maximize reward



Exploring ways to overcome vanishing gradients in RFT

Common Heuristics: Increasing learning rate, temperature, entropy regularization

Common Heuristics: Increasing learning rate, temperature, entropy regularization X

Common Heuristics: Increasing learning rate, temperature, entropy regularization X

Observation: Initial SFT phase reduces number of inputs with small reward std

Common Heuristics: Increasing learning rate, temperature, entropy regularization

Observation: Initial SFT phase reduces number of inputs with small reward std



Common Heuristics: Increasing learning rate, temperature, entropy regularization

Observation: Initial SFT phase reduces number of inputs with small reward std



① Importance of SFT in RFT pipeline: mitigates vanishing gradients

Limitation of Initial SFT Phase: Requires labeled data (5))

Limitation of Initial SFT Phase: Requires labeled data (5))

Expectation: If SFT phase is beneficial due to mitigating vanishing gradients for RFT

Limitation of Initial SFT Phase: Requires labeled data (5))

Expectation: If SFT phase is beneficial due to mitigating vanishing gradients for RFT

A few steps of SFT on small # of labeled samples should suffice

Limitation of Initial SFT Phase: Requires labeled data (5))

Expectation: If SFT phase is beneficial due to mitigating vanishing gradients for RFT

A few steps of SFT on small # of labeled samples should suffice

Result

Using **1% of labeled samples** and 40% of steps for initial SFT allows RFT to reach roughly same reward as with "full" initial SFT

Limitation of Initial SFT Phase: Requires labeled data (5))

Expectation: If SFT phase is beneficial due to mitigating vanishing gradients for RFT

A few steps of SFT on small # of labeled samples should suffice

Result

Using **1% of labeled samples** and 40% of steps for initial SFT allows RFT to reach roughly same reward as with "full" initial SFT

① The initial SFT phase does not need to be expensive!

Conclusion: Vanishing Gradients in RFT

Conclusion: Vanishing Gradients in RFT

$abla_{ heta} \mathbf{V}_{ heta}(\mathbf{x}) pprox \mathbf{0}$

Expected gradient for an input vanishes in RFT

if the input's reward std is small
Conclusion: Vanishing Gradients in RFT

 $abla_{ heta} \mathbf{V}_{ heta}(\mathbf{x}) pprox \mathbf{0}$

Expected gradient for an input vanishes in RFT if the input's reward std is small



Vanishing gradients in RFT are prevalent and detrimental to maximizing reward

Conclusion: Vanishing Gradients in RFT

 $abla_{ heta} \mathbf{V}_{ heta}(\mathbf{x}) pprox \mathbf{0}$

Expected gradient for an input vanishes in RFT if the input's reward std is small



Vanishing gradients in RFT are prevalent and detrimental to maximizing reward



Initial SFT phase allows overcoming vanishing gradients in RFT, and **does not need to be expensive**

Conclusion: Vanishing Gradients in RFT

 $abla_{ heta} \mathbf{V}_{ heta}(\mathbf{x}) pprox \mathbf{0}$

Expected gradient for an input vanishes in RFT if the input's reward std is small

Vanishing gradients in RFT are prevalent and detrimental to maximizing reward

Initial SFT phase allows overcoming vanishing gradients in RFT, and **does not need to be expensive**

O Reward std is a key quantity to track for successful RFT

Implicit Bias of Policy Gradient in Linear Quadratic Control: Extrapolation to Unseen Initial States

R + Alexander + Cohen-Karlik + Giryes + Globerson + Cohen | *arXiv* 2024

Optimal Control Problem

Optimal Control Problem

System: Starting from an initial state \mathbf{x}_0

Optimal Control Problem

System: Starting from an initial state \mathbf{x}_0 $\mathbf{x}_{h+1} = f(\mathbf{x}_h, \mathbf{u}_h)$ $h = 0, \dots, H-1$ $f(\mathbf{x}_h, \mathbf{u}_h)$ $f(\mathbf{x$

Optimal Control Problem

System: Starting from an initial state \mathbf{x}_0

 $\mathbf{x}_{h+1} = f(\mathbf{x}_h, \mathbf{u}_h) \qquad h = 0, \dots, H-1$ state control time horizon

Goal: Choose controls that minimize the cost $\sum_{h=0}^{H} c(\mathbf{x}_h, \mathbf{u}_h)$

Optimal Control Problem

$$\bigcirc$$
 System: Starting from an initial state \mathbf{x}_0

$$\mathbf{x}_{h+1} = f(\mathbf{x}_h, \mathbf{u}_h) \qquad h = 0, \dots, H-1$$

$$\texttt{state control} \qquad \texttt{time horizon}$$

Goal: Choose controls that minimize the cost $\sum_{h=0}^{H} c(\mathbf{x}_h, \mathbf{u}_h)$

Policy Gradient



(•) Parameterize controller (e.g. as neural network)

Optimal Control Problem

$$\bigcirc$$
 System: Starting from an initial state \mathbf{x}_0

$$\mathbf{x}_{h+1} = f(\mathbf{x}_h, \mathbf{u}_h) \qquad h = 0, \dots, H-1$$

$$\texttt{f} \qquad \texttt{f} \qquad \texttt{f}$$

Goal: Choose controls that minimize the cost $\sum_{h=0}^{H} c(\mathbf{x}_h, \mathbf{u}_h)$

Policy Gradient



- neural network)
- ✓ Minimize cost via gradient descent w.r.t. controller parameters

Issue of Prime Importance: Extrapolation to **initial states unseen in training**







Issue of Prime Importance: Extrapolation to **initial states unseen in training**







Often multiple controllers minimize cost for **initial states seen in training**

Issue of Prime Importance: Extrapolation to **initial states unseen in training**







Often multiple controllers minimize cost for **initial states seen in training**



Extrapolation is determined by the implicit bias of policy gradient

Issue of Prime Importance: Extrapolation to **initial states unseen in training**



Often multiple controllers minimize cost for **initial states seen in training**



Extrapolation is determined by the implicit bias of policy gradient

Effect of implicit bias on extrapolation was theoretically studied in supervised learning

(Xu et al. 2021, Abbe et al. 2022/23, Cohen-Karlik et al. 2022/23)

Issue of Prime Importance: Extrapolation to **initial states unseen in training**



Often multiple controllers minimize cost for **initial states seen in training**



Extrapolation is determined by the implicit bias of policy gradient

Effect of implicit bias on extrapolation was theoretically studied in supervised learning

(Xu et al. 2021, Abbe et al. 2022/23, Cohen-Karlik et al. 2022/23)

not understood in optimal control

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?



Theory for the Linear Quadratic Regulator (LQR) Problem: Extrapolation depends on an **interplay between the system and initial states seen in training** **Q:** To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?



Theory for the Linear Quadratic Regulator (LQR) Problem: Extrapolation depends on an interplay between the system and initial states seen in training



Experiments:

Support theory for LQR and demonstrate its conclusions apply to non-linear systems and neural network controllers

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?



Theory for the Linear Quadratic Regulator (LQR) Problem: Extrapolation depends on an **interplay between the system and initial states seen in training**



Experiments:

Support theory for LQR and demonstrate its conclusions apply to **non-linear systems and neural network controllers**

LQR Problem (state $\mathbf{x}_h \in \mathbb{R}^D$, control $\mathbf{u}_h \in \mathbb{R}^M$)

LQR Problem (state $\mathbf{x}_h \in \mathbb{R}^D$, control $\mathbf{u}_h \in \mathbb{R}^M$)

S Linear System $\mathbf{x}_{h+1} = \mathbf{A}\mathbf{x}_h + \mathbf{B}\mathbf{u}_h$







For training set of initial states $S \subset \mathbb{R}^D$ the controller is learned by minimizing the training cost:



For training set of initial states $S \subset \mathbb{R}^D$ the controller is learned by minimizing the training cost:

$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$



For training set of initial states $S \subset \mathbb{R}^D$ the controller is learned by minimizing the training cost:

$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Learning the controller via **policy gradient** amounts to:

$$\mathbf{K}^{(t+1)} = \mathbf{K}^{(t)} - \eta \cdot \nabla cost_{\mathcal{S}}(\mathbf{K}^{(t)})$$

learning rate

LQR Problem (state
$$\mathbf{x}_h \in \mathbb{R}^D$$
, control $\mathbf{u}_h \in \mathbb{R}^M$)SolutionLinear System $\mathbf{x}_{h+1} = \mathbf{A}\mathbf{x}_h + \mathbf{B}\mathbf{u}_h$ $\begin{bmatrix} \mathcal{C} \\ \mathcal{C} \\ \mathcal{D} \\ h=0 \end{bmatrix} \mathbf{x}_h^\top \mathbf{Q}\mathbf{x}_h + \mathbf{u}_h^\top \mathbf{R}\mathbf{u}_h$ $\begin{bmatrix} \mathcal{C} \\ \mathcal{C} \\ \mathcal{D} \\ h=0 \end{bmatrix} \mathbf{x}_h^\top \mathbf{Q}\mathbf{x}_h + \mathbf{u}_h^\top \mathbf{R}\mathbf{u}_h$

For training set of initial states $S \subset \mathbb{R}^D$ the controller is learned by minimizing the training cost:

$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Learning the controller via **policy gradient** amounts to:

$$\mathbf{K}^{(t+1)} = \mathbf{K}^{(t)} - \eta \cdot \nabla cost_{\mathcal{S}}(\mathbf{K}^{(t)})$$
 initialization $\mathbf{K}^{(0)} = \mathbf{0}$
learning rate

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Fraining cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Existing Analyses of Policy Gradient in LQR (e.g. Fazel et al. 2018, Malik et al. 2019, Bu et al. 2019/20)

Typically assume that:

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Existing Analyses of Policy Gradient in LQR (e.g. Fazel et al. 2018, Malik et al. 2019, Bu et al. 2019/20)

Typically assume that:

• Cost matrix **R** is positive definite – controls are regularized

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Existing Analyses of Policy Gradient in LQR (e.g. Fazel et al. 2018, Malik et al. 2019, Bu et al. 2019/20)

Typically assume that:

- Cost matrix **R** is positive definite controls are regularized
- Training set of initial states S spans \mathbb{R}^D

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Existing Analyses of Policy Gradient in LQR (e.g. Fazel et al. 2018, Malik et al. 2019, Bu et al. 2019/20)

Typically assume that:

- Cost matrix \mathbf{R} is positive definite controls are regularized
- Training set of initial states \mathcal{S} spans \mathbb{R}^D
 - Training cost has a **unique minimizer**

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Existing Analyses of Policy Gradient in LQR (e.g. Fazel et al. 2018, Malik et al. 2019, Bu et al. 2019/20)

Typically assume that:

- Cost matrix **R** is positive definite controls are regularized
- Training set of initial states \mathcal{S} spans \mathbb{R}^D
 - Training cost has a **unique minimizer**

Under these assumptions implicit bias is irrelevant

Setting: Underdetermined LQR

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Underdetermined LQR

Setting: Underdetermined LQR

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Underdetermined LQR

• $\mathbf{R} = \mathbf{0} - \text{controls}$ are not regularized
Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Underdetermined LQR

- $\mathbf{R} = \mathbf{0} \text{controls}$ are **not regularized**
- Training set of initial states S does not span \mathbb{R}^D

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Underdetermined LQR

- $\mathbf{R} = \mathbf{0} \text{controls}$ are **not regularized**
- Training set of initial states S does not span \mathbb{R}^D
- B is full rank controller's ability to affect the state is not limited

$$\mathbf{x}_{h+1} = (\mathbf{A} + \mathbf{B}\mathbf{K})\mathbf{x}_h$$

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_h^{\top} (\mathbf{Q} + \mathbf{K}^{\top} \mathbf{R} \mathbf{K}) \mathbf{x}_h$$

Underdetermined LQR

 $\mathbf{x}_{h+1} = (\mathbf{A} + \mathbf{B}\mathbf{K})\mathbf{x}_h$

- $\mathbf{R} = \mathbf{0} \text{controls}$ are **not regularized**
- Training set of initial states S does not span \mathbb{R}^D
- **B** is full rank controller's ability to affect the state is not limited

For simplicity: $\mathbf{B} = \mathbf{Q} = \mathbf{I}$

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \|\mathbf{x}_h\|^2$$

Underdetermined LQR

 $\mathbf{x}_{h+1} = (\mathbf{A} + \mathbf{B}\mathbf{K})\mathbf{x}_h$

- $\mathbf{R} = \mathbf{0} \text{controls}$ are **not regularized**
- Training set of initial states S does not span \mathbb{R}^D
- **B** is full rank controller's ability to affect the state is not limited

For simplicity: $\mathbf{B} = \mathbf{Q} = \mathbf{I}$

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \|(\mathbf{A} + \mathbf{K})^h \mathbf{x}_0\|^2$$

Underdetermined LQR

 $\mathbf{x}_{h+1} = (\mathbf{A} + \mathbf{B}\mathbf{K})\mathbf{x}_h$

- $\mathbf{R} = \mathbf{0} \text{controls}$ are **not regularized**
- Training set of initial states S does not span \mathbb{R}^D
- B is full rank controller's ability to affect the state is not limited

For simplicity: $\mathbf{B} = \mathbf{Q} = \mathbf{I}$

Training cost:
$$cost_{\mathcal{S}}(\mathbf{K}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_0 \in \mathcal{S}} \sum_{h=0}^{H} \| (\mathbf{A} + \mathbf{K})^h \mathbf{x}_0 \|^2$$

Underdetermined LQR

- $\mathbf{R} = \mathbf{0} \text{controls}$ are **not regularized**
- Training set of initial states S does not span \mathbb{R}^D

For simplicity: $\mathbf{B} = \mathbf{Q} = \mathbf{I}$

• **B** is full rank – controller's ability to affect the state is not limited $\mathbf{x}_{h+1} = (\mathbf{A} + \mathbf{B}\mathbf{K})\mathbf{x}_h$

In this setting the training cost has multiple minimizers

Optimality Condition: K minimizes the training cost if and only if $||(\mathbf{A} + \mathbf{K})\mathbf{x}_0||^2 = 0$ for all $\mathbf{x}_0 \in S$

Optimality Condition: K minimizes the training cost if and only if $\|(\mathbf{A} + \mathbf{K})\mathbf{x}_0\|^2 = 0$ for all $\mathbf{x}_0 \in S$

 \mathbf{K} sends \mathbf{x}_0 to zero

Optimality Condition: K minimizes the training cost if and only if $\|(A + K)x_0\|^2 = 0$ for all $x_0 \in S$

 $\mathbf K$ sends $\mathbf x_0$ to zero

Let ${\mathcal U}$ be an arbitrary orthonormal basis of ${\mathcal S}^\perp$

Optimality Condition: K minimizes the training cost if and only if $\|(\mathbf{A} + \mathbf{K})\mathbf{x}_0\|^2 = 0$ for all $\mathbf{x}_0 \in S$

 ${\bf K}$ sends ${\bf x}_0$ to zero

Let $\mathcal U$ be an arbitrary orthonormal basis of $\mathcal S^{\perp}$

Controllers minimizing the training cost

Optimality Condition: K minimizes the training cost if and only if $\|(\mathbf{A} + \mathbf{K})\mathbf{x}_0\|^2 = 0$ for all $\mathbf{x}_0 \in S$



Let ${\mathcal U}$ be an arbitrary orthonormal basis of ${\mathcal S}^\perp$

Controllers minimizing the training cost 🗸

- produce **identical controls** for states in S

differ arbitrarily in their controls for states in $\ensuremath{\mathcal{U}}$

Optimality Condition: K minimizes the training cost if and only if $\|(A + K)x_0\|^2 = 0$ for all $x_0 \in S$



Let ${\mathcal U}$ be an arbitrary orthonormal basis of ${\mathcal S}^\perp$

Controllers minimizing the training cost $\begin{cases} produce identical controls for states in S \\ differ arbitrarily in their controls for states in U \end{cases}$

We quantify extrapolation for a controller ${\bf K}$ by its performance on initial states in ${\cal U}$

Optimality Condition: K minimizes the training cost if and only if $\|(\mathbf{A} + \mathbf{K})\mathbf{x}_0\|^2 = 0$ for all $\mathbf{x}_0 \in S$



Let ${\mathcal U}$ be an arbitrary orthonormal basis of ${\mathcal S}^\perp$

Controllers minimizing the training cost $\begin{cases} produce identical controls for states in S \\ differ arbitrarily in their controls for states in U \end{cases}$

We quantify extrapolation for a controller ${\bf K}$ by its performance on initial states in ${\cal U}$

Extrapolation Error

$$\mathcal{E}(\mathbf{K}) := \frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_0 \in \mathcal{U}} \| (\mathbf{A} + \mathbf{K}) \mathbf{x}_0 \|^2$$

Extrapolation Error

$$\mathcal{E}(\mathbf{K}) := \frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_0 \in \mathcal{U}} \|(\mathbf{A} + \mathbf{K}) \mathbf{x}_0 \|^2$$

Extrapolation Error

$$\mathcal{E}(\mathbf{K}) := \frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_0 \in \mathcal{U}} \|(\mathbf{A} + \mathbf{K}) \mathbf{x}_0 \|^2$$

Perfectly Extrapolating \mathbf{K}_{ext}

Extrapolation Error

$$\mathcal{E}(\mathbf{K}) := \frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_0 \in \mathcal{U}} \|(\mathbf{A} + \mathbf{K}) \mathbf{x}_0 \|^2$$

Perfectly Extrapolating \mathbf{K}_{ext}

Satisfies $(\mathbf{A} + \mathbf{K}_{ext})\mathbf{x}_0 = \mathbf{0}$ for all $\mathbf{x}_0 \in \mathbb{R}^D$

Extrapolation Error

$$\mathcal{E}(\mathbf{K}) := \frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_0 \in \mathcal{U}} \|(\mathbf{A} + \mathbf{K}) \mathbf{x}_0 \|^2$$

Perfectly Extrapolating \mathbf{K}_{ext}

Satisfies $(\mathbf{A} + \mathbf{K}_{ext})\mathbf{x}_0 = \mathbf{0}$ for all $\mathbf{x}_0 \in \mathbb{R}^D$

Minimizes the training cost and $\mathcal{E}(\mathbf{K}_{ext}) = 0$

Extrapolation Error

$$\mathcal{E}(\mathbf{K}) := \frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_0 \in \mathcal{U}} \|(\mathbf{A} + \mathbf{K}) \mathbf{x}_0\|^2$$

Perfectly Extrapolating \mathbf{K}_{ext}

Satisfies $(\mathbf{A} + \mathbf{K}_{ext})\mathbf{x}_0 = \mathbf{0}$ for all $\mathbf{x}_0 \in \mathbb{R}^D$

Minimizes the training cost and $\mathcal{E}(\mathbf{K}_{\mathrm{ext}}) = 0$

Non-Extrapolating $\mathbf{K}_{no\text{-ext}}$

Extrapolation Error

$$\mathcal{E}(\mathbf{K}) := \frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_0 \in \mathcal{U}} \|(\mathbf{A} + \mathbf{K}) \mathbf{x}_0\|^2$$

Perfectly Extrapolating \mathbf{K}_{ext}

Satisfies $(\mathbf{A} + \mathbf{K}_{ext})\mathbf{x}_0 = \mathbf{0}$ for all $\mathbf{x}_0 \in \mathbb{R}^D$

Minimizes the training cost and $\mathcal{E}(\mathbf{K}_{\mathrm{ext}}) = 0$

Non-Extrapolating $\mathbf{K}_{no\text{-ext}}$

$$\mathsf{Satisfies}\,(\mathbf{A} + \mathbf{K}_{\mathrm{no-ext}})\mathbf{x}_0 = \begin{cases} \mathbf{0} &, \mathbf{x}_0 \in \mathcal{S} \\ \mathbf{A}\mathbf{x}_0 &, \mathbf{x}_0 \in \mathcal{U} \end{cases}$$

Extrapolation Error

$$\mathcal{E}(\mathbf{K}) := \frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_0 \in \mathcal{U}} \|(\mathbf{A} + \mathbf{K}) \mathbf{x}_0 \|^2$$

Perfectly Extrapolating \mathbf{K}_{ext}

Satisfies $(\mathbf{A} + \mathbf{K}_{ext})\mathbf{x}_0 = \mathbf{0}$ for all $\mathbf{x}_0 \in \mathbb{R}^D$

Minimizes the training cost and $\mathcal{E}(\mathbf{K}_{\mathrm{ext}}) = 0$

Non-Extrapolating $\mathbf{K}_{no\text{-ext}}$

$$\mathsf{Satisfies} \left(\mathbf{A} + \mathbf{K}_{\mathrm{no-ext}} \right) \mathbf{x}_0 = \begin{cases} \mathbf{0} & , \mathbf{x}_0 \in \mathcal{S} \\ \mathbf{A} \mathbf{x}_0 & , \mathbf{x}_0 \in \mathcal{U} \end{cases}$$

Minimizes the training cost but $\mathcal{E}(\mathbf{K}_{no\text{-}\mathrm{ext}}) \text{ is typically high}$



- initial state seen in training
- state explored during policy gradient
- state unexplored during policy gradient



- initial state seen in training
- state explored during policy gradient
- state unexplored during policy gradient



- initial state seen in training
- state explored during policy gradient
- state unexplored during policy gradient

 $\mathbf{K}^{(t)}$ - the policy gradient controller $\begin{array}{c} \mathcal{S} & - \text{ initial states seen} \\ & \text{ at iteration } t \end{array}$ in training

 $\begin{array}{lll} \mathbf{K}^{(t)} - \text{the policy gradient controller} & \mathcal{S} - \text{initial states seen} & \mathcal{X}_{pg} - \text{the set of states encountered} \\ & \text{at iteration } t & \text{in training} & \text{during policy gradient} \end{array}$

 $\begin{array}{lll} \mathbf{K}^{(t)} - \text{the policy gradient controller} & \mathcal{S} - \text{initial states seen} & \mathcal{X}_{pg} - \text{the set of states encountered} \\ & \text{at iteration } t & \text{in training} & \text{during policy gradient} \end{array}$

Proposition – Exploration is Necessary for Extrapolation

 $\begin{array}{lll} \mathbf{K}^{(t)} - \text{the policy gradient controller} & \mathcal{S} - \text{initial states seen} & \mathcal{X}_{pg} - \text{the set of states encountered} \\ & \text{at iteration } t & \text{in training} & \text{during policy gradient} \end{array}$

Proposition – Exploration is Necessary for Extrapolation

• For any $\mathbf{x} \in \mathcal{X}_{pg}^{\perp}$ the controls produced by $\mathbf{K}^{(t)}$ and \mathbf{K}_{no-ext} are the same

 $\begin{array}{lll} \mathbf{K}^{(t)} - \text{the policy gradient controller} & \mathcal{S} - \text{initial states seen} & \mathcal{X}_{pg} - \text{the set of states encountered} \\ & \text{at iteration } t & \text{in training} & \text{during policy gradient} \end{array}$

Proposition – Exploration is Necessary for Extrapolation

- For any $\mathbf{x} \in \mathcal{X}_{pg}^{\perp}$ the controls produced by $\mathbf{K}^{(t)}$ and \mathbf{K}_{no-ext} are the same
- There exist systems s.t. $\mathcal{X}_{pg} \subseteq \operatorname{span}(\mathcal{S})$ and $\mathcal{E}(\mathbf{K}^{(t)}) = \mathcal{E}(\mathbf{K}_{no-ext})$

Q: Exploration is necessary for extrapolation, but can it be sufficient?

Q: Exploration is necessary for extrapolation, but can it be sufficient? 🕗

Q: Exploration is necessary for extrapolation, but can it be sufficient? 🕗

Simple "Shift" Setting

- Consider training initial state \mathbf{e}_1
 - first standard basis vector

Q: Exploration is necessary for extrapolation, but can it be sufficient? 🕗

Simple "Shift" Setting

- Consider training initial state \mathbf{e}_1
 - first standard basis vector
- The trajectory steered by $\mathbf{K}^{(0)}$ is $\mathbf{e}_1, \mathbf{A}\mathbf{e}_1, \dots, \mathbf{A}^{H-1}\mathbf{e}_1$

Q: Exploration is necessary for extrapolation, but can it be sufficient? 📀

Simple "Shift" Setting

- Consider training initial state e₁
 first standard basis vector
- The trajectory steered by $\mathbf{K}^{(0)}$ is $\mathbf{e}_1, \mathbf{A}\mathbf{e}_1, \dots, \mathbf{A}^{H-1}\mathbf{e}_1$

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$

Ensures trajectory spans whole state space
Extrapolation in Exploration-Inducing Setting

Q: Exploration is necessary for extrapolation, but can it be sufficient? 🕗

Simple "Shift" Setting

- Consider training initial state e₁
 first standard basis vector
- The trajectory steered by $\mathbf{K}^{(0)}$ is $\mathbf{e}_1, \mathbf{A}\mathbf{e}_1, \dots, \mathbf{A}^{H-1}\mathbf{e}_1$

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$

 $\begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 1 \end{pmatrix}$

Ensures trajectory spans whole state space

Proposition

Policy gradient converges to \mathbf{K}_{pg} , which minimizes the training cost and:

 $\mathcal{E}(\mathbf{K}_{\mathrm{pg}}) <\!\!< \mathcal{E}(\mathbf{K}_{\mathrm{no-ext}})$

Extrapolation in Exploration-Inducing Setting

Q: Exploration is necessary for extrapolation, but can it be sufficient? 📀

Simple "Shift" Setting

- Consider training initial state e₁
 first standard basis vector
- The trajectory steered by $\mathbf{K}^{(0)}$ is $\mathbf{e}_1, \mathbf{A}\mathbf{e}_1, \dots, \mathbf{A}^{H-1}\mathbf{e}_1$

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$

 $\begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 1 \end{pmatrix}$

Ensures trajectory spans whole state space

Proposition

Policy gradient converges to \mathbf{K}_{pg} , which minimizes the training cost and:

 $\mathcal{E}(\mathbf{K}_{\rm pg}) <\!\!< \mathcal{E}(\mathbf{K}_{\rm no\text{-}ext})$

where perfect extrapolation is attained when the horizon $H \to \infty$

Q: We saw two ends of a spectrum, but which type of extrapolation do we typically get?

Q: We saw two ends of a spectrum, but which type of extrapolation do we typically get?

Typical Setting

• Arbitrary training initial state \mathbf{x}_0

Q: We saw two ends of a spectrum, but which type of extrapolation do we typically get?

state dimension

30/38

Typical Setting

- Arbitrary training initial state \mathbf{x}_0
- Random A with entries sampled indepently from $\mathcal{N}(0, 1/D)$

Q: We saw two ends of a spectrum, but which type of extrapolation do we typically get?

30/38

Typical Setting

- Arbitrary training initial state \mathbf{x}_0
- Random A with entries sampled indepently from $\mathcal{N}(0, 1/D)$

Theorem

If the learning rate η is sufficiently small, a single iteration of policy gradient leads to non-trivial extrapolation:

state dimension

Q: We saw two ends of a spectrum, but which type of extrapolation do we typically get?

Typical Setting

- Arbitrary training initial state \mathbf{x}_0
- Random A with entries sampled indepently from $\mathcal{N}(0, 1/D)$

Theorem

If the learning rate η is sufficiently small, a single iteration of policy gradient leads to non-trivial extrapolation:

$$\mathbb{E}\left[\mathcal{E}(\mathbf{K}^{(1)})\right] \leq \mathbb{E}\left[\mathcal{E}(\mathbf{K}_{\text{no-ext}})\right] - \Omega\left(\eta \cdot \frac{H^2}{D}\right)$$

state dimension

Q: We saw two ends of a spectrum, but which type of extrapolation do we typically get?

Typical Setting

- Arbitrary training initial state \mathbf{x}_0
- Random A with entries sampled indepently from $\mathcal{N}(0, 1/D)$

Theorem

If the learning rate η is sufficiently small, a single iteration of policy gradient leads to non-trivial extrapolation:

$$\mathbb{E}\left[\mathcal{E}(\mathbf{K}^{(1)})\right] \leq \mathbb{E}\left[\mathcal{E}(\mathbf{K}_{\text{no-ext}})\right] - \Omega\left(\eta \cdot \frac{H^2}{D}\right)$$

Additionally, extrapolation occurs with high probability if D is large

state dimension

Theorem

If the learning rate η is sufficiently small, a single iteration of policy gradient leads to non-trivial extrapolation:

$$\mathbb{E}\left[\mathcal{E}(\mathbf{K}^{(1)})\right] \leq \mathbb{E}\left[\mathcal{E}(\mathbf{K}_{\text{no-ext}})\right] - \Omega\left(\eta \cdot \frac{H^2}{D}\right)$$

Additionally, extrapolation occurs with high probability if D is large

Proof Idea:

Theorem

If the learning rate η is sufficiently small, a single iteration of policy gradient leads to non-trivial extrapolation:

$$\mathbb{E}\left[\mathcal{E}(\mathbf{K}^{(1)})\right] \leq \mathbb{E}\left[\mathcal{E}(\mathbf{K}_{\text{no-ext}})\right] - \Omega\left(\eta \cdot \frac{H^2}{D}\right)$$

Additionally, extrapolation occurs with high probability if D is large

Proof Idea:

• Intuition: Random system generically induces exploration

Theorem

If the learning rate η is sufficiently small, a single iteration of policy gradient leads to non-trivial extrapolation:

$$\mathbb{E}\left[\mathcal{E}(\mathbf{K}^{(1)})\right] \leq \mathbb{E}\left[\mathcal{E}(\mathbf{K}_{\text{no-ext}})\right] - \Omega\left(\eta \cdot \frac{H^2}{D}\right)$$

Additionally, extrapolation occurs with high probability if D is large

Proof Idea:

- Intuition: Random system generically induces exploration
- Convert intuition to formal guarantee via tools from random matrix theory and topology

Theorem

If the learning rate η is sufficiently small, a single iteration of policy gradient leads to non-trivial extrapolation:

$$\mathbb{E}\left[\mathcal{E}(\mathbf{K}^{(1)})\right] \leq \mathbb{E}\left[\mathcal{E}(\mathbf{K}_{\text{no-ext}})\right] - \Omega\left(\eta \cdot \frac{H^2}{D}\right)$$

Additionally, extrapolation occurs with high probability if D is large

Proof Idea:

- Intuition: Random system generically induces exploration
- Convert intuition to formal guarantee via tools from random matrix theory and topology

Limitations: Condition on learning rate + only second iterate of policy gradient

Theorem

If the learning rate η is sufficiently small, a single iteration of policy gradient leads to non-trivial extrapolation:

$$\mathbb{E}\left[\mathcal{E}(\mathbf{K}^{(1)})\right] \leq \mathbb{E}\left[\mathcal{E}(\mathbf{K}_{\text{no-ext}})\right] - \Omega\left(\eta \cdot \frac{H^2}{D}\right)$$

Additionally, extrapolation occurs with high probability if D is large

Proof Idea:

- Intuition: Random system generically induces exploration
- Convert intuition to formal guarantee via tools from random matrix theory and topology

Limitations: Condition on learning rate + only second iterate of policy gradient

experiments suggest these limitations may be alleviated

Supervised Learning



Task: Linear regression

Known (e.g. Zhang et al. 2017): Implicit bias minimizes **Euclidean norm**







Corollary

Among controllers minimizing the training cost, $\mathbf{K}_{\mathrm{no-ext}}$ has the minimal Euclidean norm



Corollary

Among controllers minimizing the training cost, $K_{\rm no\text{-}ext}$ has the minimal Euclidean norm



Extrapolation implies policy gradient does not implicitly minimize Euclidean norm

Main Contributions: Effect of Implicit Bias on Extrapolation

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?



Theory for the Linear Quadratic Regulator (LQR) Problem: Extrapolation depends on an **interplay between the system and initial states seen in training**



Experiments:

Support theory for LQR and demonstrate its conclusions apply to non-linear systems and neural network controllers

Experiments: Analyzed LQR Problems

Experiments: Analyzed LQR Problems



Experiments: Analyzed LQR Problems



In accordance with our theory:

In the extrapolation occurs under the identity system, while for the shift and random systems we have non-trivial extrapolation (yet not perfect)

Our Theory: Linear system induces exploration from initial states seen in training

Our Theory: Linear system induces exploration from initial states seen in training \longrightarrow Linear controller typically extrapolates

Our Theory: Linear system induces exploration from initial states seen in training \longrightarrow Linear controller typically extrapolates **Experiments:** Phenomenon extends to **non-linear systems** and **neural network controllers**

Our Theory: Linear system induces exploration from initial states seen in training \longrightarrow Linear controller typically extrapolates **Experiments:** Phenomenon extends to **non-linear systems** and **neural network controllers**

Pendulum Control Problem

(analogous experiments for a quadcopter control problem)

Our Theory: Linear system induces exploration from initial states seen in training \longrightarrow Linear controller typically extrapolates **Experiments:** Phenomenon extends to **non-linear systems** and **neural network controllers**

Pendulum Control Problem

(analogous experiments for a quadcopter control problem)

- 🛧 target state
- initial state seen in training
- initial state unseen in training



Our Theory: Linear system induces exploration from initial states seen in training \longrightarrow Linear controller typically extrapolates **Experiments:** Phenomenon extends to **non-linear systems** and **neural network controllers**

Pendulum Control Problem

(analogous experiments for a quadcopter control problem)

- 🛧 target state
- initial state seen in training
- initial state unseen in training



Our Theory: Linear system induces exploration from initial states seen in training \longrightarrow Linear controller typically extrapolates **Experiments:** Phenomenon extends to **non-linear systems** and **neural network controllers**

Pendulum Control Problem

(analogous experiments for a quadcopter control problem)

🛧 target state

• initial state seen in training

• initial state unseen in training



Our Theory: Linear system induces exploration from initial states seen in training \longrightarrow Linear controller typically extrapolates **Experiments:** Phenomenon extends to **non-linear systems** and **neural network controllers**

Pendulum Control Problem

(analogous experiments for a quadcopter control problem)

🛧 target state

• initial state seen in training

• initial state unseen in training



① The controller learned via policy gradient extrapolates despite existence of non-extrapolating controllers

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?

36/38



Theory for the LQR Problem:

Extrapolation depends on exploration induced by the system from initial states seen in training

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?



Theory for the LQR Problem:

Extrapolation depends on exploration induced by the system from initial states seen in training



Experiments: Support theory for LQR and demonstrate its conclusions apply to non-linear systems and neural network controllers

36/38

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?



Theory for the LQR Problem:

Extrapolation depends on exploration induced by the system from initial states seen in training

Going Forward:



Experiments: Support theory for LQR and demonstrate its conclusions apply to non-linear systems and neural network controllers
Conclusion: Implicit Bias of Policy Gradient in Optimal Control

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?



Theory for the LQR Problem: Extrapolation depends on exploration induced by the system

from initial states seen in training

Going Forward:

• Theory for non-linear systems and neural network controllers



Experiments: Support theory for LQR and demonstrate its conclusions apply to **non-linear systems and neural network controllers**

Conclusion: Implicit Bias of Policy Gradient in Optimal Control

Q: To what extent does the implicit bias of policy gradient lead to extrapolation to initial states unseen in training?



Theory for the LQR Problem: Extrapolation depends on exploration induced by the system from initial states seen in training

Experiments: Support theory for LQR and demonstrate its conclusions apply to **non-linear systems and neural network controllers**

Going Forward:

- Theory for non-linear systems and neural network controllers
- Enhancing extrapolation via methods for selecting initial states to train on

Outlook

Supervised Learning



Optimization and implicit bias have been extensively studied

Supervised Learning



Optimization and implicit bias have been extensively studied

Optimal Control/Reinforcement Learning



Our Results: Optimization and implicit bias can substantially differ from those in supervised learning, hence require dedicated study

Supervised Learning



Optimization and implicit bias have been extensively studied

Optimal Control/Reinforcement Learning



Our Results: Optimization and implicit bias can substantially differ from those in supervised learning, hence require dedicated study

① Studying optimization and implicit bias in optimal control/reinforcement learning may allow addressing their unique challenges

Thank You!

Work supported by:

Apple scholars in AI/ML PhD fellowship, Google Research Scholar Award, Google Research Gift, the Yandex Initiative in Machine Learning, the Israel Science Foundation (grant 1780/21), Len Blavatnik and the Blavatnik Family Foundation, Tel Aviv University Center for AI and Data Science, and Amnon and Anat Shashua