# Analyses of Policy Gradient for Language Model Finetuning and Optimal Control 

Noam Razin
Tel Aviv University

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## Optimization and Generalization in Modern Machine Learning

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Optimization

Minimize a non-convex training objective

## Optimization and Generalization in Modern Machine Learning



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## Optimization and Generalization in Modern Machine Learning



Generalization


Performance on data unseen in training


Determined by implicit bias of training algorithm

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

## Supervised Learning vs Optimal Control/Reinforcement Learning

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Supervised Learning


Task: Learn predictor minimizing loss over labeled data

Training Algorithm: Gradient descent

## Supervised Learning vs Optimal Control/Reinforcement Learning



[^0]
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Task: Learn predictor minimizing loss over labeled data

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Optimization Dynamics and Implicit Bias Extensively Studied

## Optimal Control/Reinforcement Learning



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

Training Algorithm: Policy gradient

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Optimization Dynamics and Implicit Bias Limited Understanding
(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)

Sources

## Optimization

## Implicit Bias

Vanishing Gradients in Reinforcement Finetuning of Language Models

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

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 

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softmax is used for producing next-token probabilities

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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)

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## Main Contributions: Vanishing Gradients in RFT

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& \text { Fundamental vanishing gradients } \\
& \text { problem in RFT }
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## Vanishing Gradients Due to Small Reward Standard Deviation (STD)

$\mathrm{STD}_{\mathrm{y} \sim p_{\theta}(\cdot \mid \mathrm{x})}[r(\mathrm{x}, \mathrm{y})]$ - reward std of x under the model

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Can be problematic when finetuning text distribution differs from pretraining

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Vanishing gradients are prevalent and harm ability to maximize reward

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

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NarrativeQA (many inputs w/ small std)

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NarrativeQA
(train)



## Overcoming Vanishing Gradients in RFT

Common Heuristics: Increasing learning rate, temperature, entropy regularization

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(1) Importance of SFT in RFT pipeline: mitigates vanishing gradients

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() The initial SFT phase does not need to be expensive!

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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
(1) 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

## Policy Gradient in Optimal Control

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

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Policy Gradient
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Policy Gradient
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$\nabla$ Minimize cost via gradient descent w.r.t. controller parameters

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Issue of Prime Importance: Extrapolation
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## Main Contributions: Effect of Implicit Bias on Extrapolation

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

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$\left(\begin{array}{ccc}0 & 1 & 0 . . . . . \\ 10 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 1 & 0\end{array}\right) \quad$ Theory for the Linear Quadratic Regulator (LQR) Problem:
Extrapolation depends on an interplay between the system and initial states seen in training

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## Experiments:

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

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> © Quadratic Costs
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กัㅇํ Linear Controller

$$
\mathbf{u}_{h}=\mathbf{K} \mathbf{x}_{h}
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\% Linear Controller

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

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& \mathbf{x}_{h+1}=\mathbf{A} \mathbf{x}_{h}+\mathbf{B} \mathbf{u}_{h}
\end{aligned} \quad \begin{gathered}
\text { C } \text { Quadratic Costs } \\
\sum_{h=0}^{H} \mathbf{x}_{h}^{\top} \mathbf{Q} \mathbf{x}_{h}+\mathbf{u}_{h}^{\top} \mathbf{R} \mathbf{u}_{h}
\end{gathered}
$$

(\%) Linear Controller

$$
\mathbf{u}_{h}=\mathbf{K} \mathbf{x}_{h}
$$

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

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\operatorname{cost}_{\mathcal{S}}(\mathbf{K})=\frac{1}{|\mathcal{S}|} \sum_{\mathbf{x}_{0} \in \mathcal{S}} \sum_{h=0}^{H} \mathbf{x}_{h}^{\top}\left(\mathbf{Q}+\mathbf{K}^{\top} \mathbf{R K}\right) \mathbf{x}_{h}
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## The Linear Quadratic Regulator (LQR) Problem

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

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Learning the controller via policy gradient amounts to:

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

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Training cost has a unique minimizer
Under these assumptions implicit bias is irrelevant

## Setting: Underdetermined LQR

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```
\mp@subsup{x}{h+1}{}}=(\mathbf{A}+\mathbf{BK})\mp@subsup{\mathbf{x}}{h}{
```

In this setting the training cost has multiple minimizers

# Quantifying Extrapolation 

## Quantifying Extrapolation

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

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K sends $\mathrm{x}_{0}$ to zero
Let $\mathcal{U}$ be an arbitrary orthonormal basis of $\mathcal{S}^{\perp}$

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Controllers minimizing the training cost

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$K$ sends $\mathbf{x}_{0}$ to zero
Let $\mathcal{U}$ be an arbitrary orthonormal basis of $\mathcal{S}^{\perp}$
Controllers minimizing the training cost $\left\{\begin{array}{l}\text { produce identical controls for states in } \mathcal{S} \\ \text { differ arbitrarily in their controls for states in } \mathcal{U}\end{array}\right.$

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## Extrapolation Error

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\mathcal{E}(\mathbf{K}):=\frac{1}{|\mathcal{U}|} \sum_{\mathbf{x}_{0} \in \mathcal{U}}\left\|(\mathbf{A}+\mathbf{K}) \mathbf{x}_{0}\right\|^{2}
$$

# Quantifying Extrapolation: Baseline Controllers 

- 

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

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Minimizes the training cost and

$$
\mathcal{E}\left(\mathbf{K}_{\mathrm{ext}}\right)=0
$$

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

$$
\text { Satisfies }\left(\mathbf{A}+\mathbf{K}_{\text {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}
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## Intuition: Extrapolation Depends on Exploration

Intuition Behind Our Analysis: Extrapolation depends on degree of exploration induced by the system from training initial states

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Policy Gradient Iterate $t$ Controller
State Dynamics: A $+\mathbf{K}^{(t)}$


- initial state seen in training
- state explored during policy gradient
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Policy Gradient Final Controller
State Dynamics: A $+\mathbf{K}_{\mathrm{pg}}$


- initial state seen in training
- state explored during policy gradient
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$\mathbf{K}^{(t)}$ - the policy gradient controller at iteration $t$
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Proposition - Exploration is Necessary for Extrapolation

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Proposition - Exploration is Necessary for Extrapolation

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


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Proposition - Exploration is Necessary for Extrapolation

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


## Extrapolation in Exploration-Inducing Setting

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

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is $\mathbf{e}_{1}, \mathbf{A} \mathbf{e}_{1}, \ldots, \mathbf{A}^{H-1} \mathbf{e}_{1}$


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$$
\longrightarrow \mathbf{A}=\left(\begin{array}{cccccc}
0 & 0 & 0 & \cdots & 0 & 1 \\
1 & 0 & 0 & \cdots & 0 & 0 \\
0 & 1 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & 0
\end{array}\right)
$$

Ensures trajectory spans whole state space

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## Proposition

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

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

## Extrapolation in Typical Setting

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

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- Random $\mathbf{A}$ with entries sampled indepently from $\mathcal{N}(0,1 / D)$


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## Theorem

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

## Extrapolation in Typical Setting

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

## Typical Setting

- Arbitrary training initial state $\mathbf{x}_{0}$

> state dimension

- Random $\mathbf{A}$ with entries sampled indepently from $\mathcal{N}(0,1 / D)$


## Theorem

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\mathbb{E}\left[\mathcal{E}\left(\mathbf{K}^{(1)}\right)\right] \leq \mathbb{E}\left[\mathcal{E}\left(\mathbf{K}_{\mathrm{no}-\mathrm{ext}}\right)\right]-\Omega\left(\eta \cdot \frac{H^{2}}{D}\right)
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Additionally, extrapolation occurs with high probability if $D$ is large

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Limitations: Condition on learning rate + only second iterate of policy gradient
experiments suggest these limitations may be alleviated

## Implicit Bias in Optimal Control $=$ E Euclidean Norm Minimization

$\square$

Supervised Learning


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

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

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## Corollary

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

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## Experiments: Analyzed LQR Problems



In accordance with our theory:
(1) No extrapolation occurs under the identity system, while for the shift and random systems we have non-trivial extrapolation (yet not perfect)

## Experiments: Non-Linear Systems and Neural Network Controllers

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(analogous experiments for a
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$\approx$ target state

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Initial States (time step 0)


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Policy Gradient Controller Final States (time step 100)


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Non-Extrapolating Controller
Final States (time step 100)


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Policy Gradient Controller

Final States (time step 100)


Non-Extrapolating Controller
Final States (time step 100)

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

## Conclusion: Implicit Bias of Policy Gradient in Optimal Control

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$\left(\begin{array}{cccc}0 & 1 & 0 & \cdots \\ 1 & 1 & \ldots \\ 0 & 1 & \ldots & 1 \\ 0 & 1 & \ldots \\ 0 & 1 & 0 & 0 \\ 0 & 1 & \cdots & 1\end{array}\right)$
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- Theory for non-linear systems and neural network controllers
- Enhancing extrapolation via methods for selecting initial states to train on


## Outlook

## Optimization and Implicit Bias in Optimal Control/Reinforcement Learning

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## Supervised Learning



Optimization and implicit bias have been extensively studied

## Optimization and Implicit Bias in Optimal Control/Reinforcement 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

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## 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!

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[^0]:    (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)

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