Optimization Challenges in Adversarial Machine Learning

EPFL CIS - RIKEN AIP Joint Seminar Series

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- DS3 Summer School Lectures

Today: “Basic” adversarial machine learning in 45mins

$$\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y})$$

- A seemingly simple optimization formulation
- Critical in machine learning with many applications
  - Adversarial examples and training
  - Generative adversarial networks
  - Robust reinforcement learning

Warm up: Flexibility of the template

$$\Phi^\star = \min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y}) \quad (\text{argmin}, \text{argmax} \to \mathbf{x}^\star, \mathbf{y}^\star)$$

Warm up: Flexibility of the template

$$\Phi^\star = \min_{\mathbf{x}\in\mathcal{X}} \underbrace{\max_{\mathbf{y}:\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y})}_{f(\mathbf{x})} \quad (\text{argmin}, \text{argmax} \to \mathbf{x}^\star, \mathbf{y}^\star)$$

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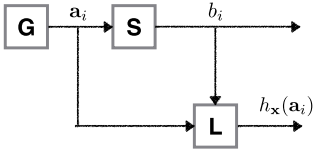
- (eula) In the sequel,
  - the set $\mathcal{X}$ is convex and has a tractable projection operator $\pi_{\mathcal{X}}$
  - all convergence characterizations are with feasible iterates $\mathbf{x}^k \in \mathcal{X}$
  - gradient mapping means $G_\alpha(\mathbf{x}^k) = \frac{1}{\alpha}[\mathbf{x}^k - \pi_{\mathcal{X}}(\mathbf{x}^k - \alpha\nabla f(\mathbf{x}^k))]$, where α is the step-size
  - L-smooth means $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L\|\mathbf{x}-\mathbf{y}\|, \forall \mathbf{x},\mathbf{y} \in \mathcal{X}$
  - ∂ may refer to the generalized subdifferential, and $\delta_{\mathcal{X}}$ refers to the indicator function for the set $\mathcal{X}$

A deep learning optimization problem in supervised learning



Definition (Optimization formulation)

The deep-learning training problem is given by

$$\mathbf{x}_{\mathsf{DL}}^{\star} \in \arg\min_{\mathbf{x}\in\mathcal{X}} \left\{ f(\mathbf{x}) := \frac{1}{n}\sum_{i=1}^{n} L(h_{\mathbf{x}}(\mathbf{a}_i), b_i) \right\},$$

where $\mathcal{X}$ denotes the constraints on the parameters.

Some frequently used loss functions

- $L(h_{\mathbf{x}}(\mathbf{a}), b) = \log(1 + \exp(-b h_{\mathbf{x}}(\mathbf{a})))$ *logistic loss*
- $L(h_{\mathbf{x}}(\mathbf{a}), b) = (b - h_{\mathbf{x}}(\mathbf{a}))^2$ *squared error*
- $L(h_{\mathbf{x}}(\mathbf{a}), b) = \max(0, 1 - b h_{\mathbf{x}}(\mathbf{a}))$ *hinge loss*

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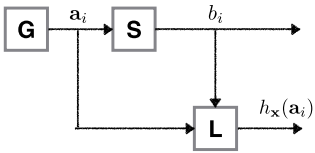

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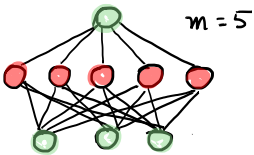
where $\mathcal{X}$ denotes the constraints on the parameters.

- A single hidden layer neural network with params $\mathbf{x} := [\mathbf{X}_1, \mathbf{X}_2, \mu_1, \mu_2]$



$$h_{\mathbf{x}}(\mathbf{a}) := \begin{bmatrix} \mathbf{X}_2 \end{bmatrix} \sigma \left(\begin{bmatrix} \mathbf{X}_1 \end{bmatrix} \begin{bmatrix} \mathbf{a} \end{bmatrix} + \begin{bmatrix} \mu_1 \end{bmatrix} \right) + \begin{bmatrix} \mu_2 \end{bmatrix}$$

activation ↓ σ | weight ↓ $\mathbf{X}_1$ | input ↓ $\mathbf{a}$ | bias ↓ μ_1 | bias ↓ μ_2

hidden layer = learned features

An approximation theoretic motivation: Why neural networks?

Theorem (Universal approximation [4])

Let $\sigma(\cdot)$ be a nonconstant, bounded, and increasing continuous function. Let $I_d = [0,1]^d$. The space of continuous functions on I_d is denoted by $\mathcal{C}(I_d)$.

Given $\epsilon > 0$ and $g \in \mathcal{C}(I_d)$ there exists a 1-hidden-layer network h with m neurons such that h is an ϵ-approximation of g, i.e.,

$$\sup_{\mathbf{a} \in I_d} |g(\mathbf{a}) - h(\mathbf{a})| \leq \epsilon$$

Caveat

The number of neurons m needed to approximate some function g can be arbitrarily large!

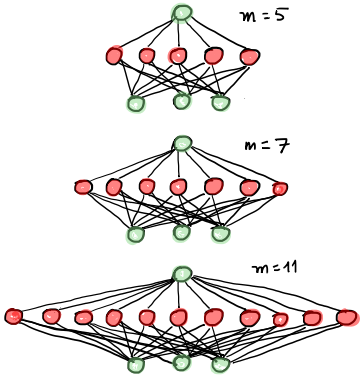
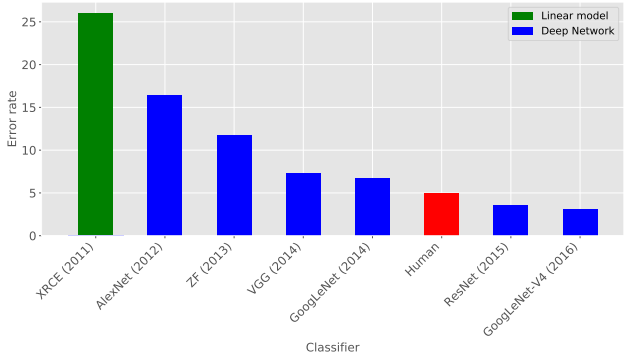


Figure: Neural networks of increasing width

A more realistic motivation: Why neural networks?

- Practical performance in applications



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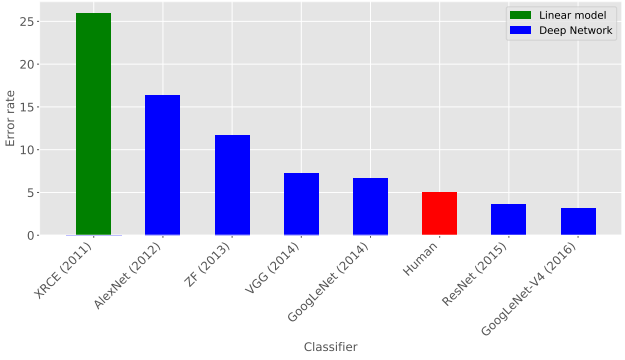


- The human: Andrej Karpathy[1]

[1] https://karpathy.github.io/2014/09/02/what-i-learned-from-competing-against-a-convnet-on-imagenet/

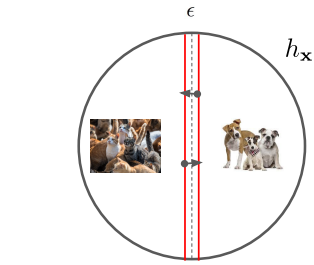
A grand challenge in DL/ML applications: Robustness (I)

(a) Turtle classified as rifle. Athalye et al. 2018.

(b) Stop sign classified as 45 mph sign. Eykholt et al. 2018

Figure: Natural or human-crafted modifications that trick neural networks used in computer vision tasks

A grand challenge in DL/ML applications: Robustness (II)



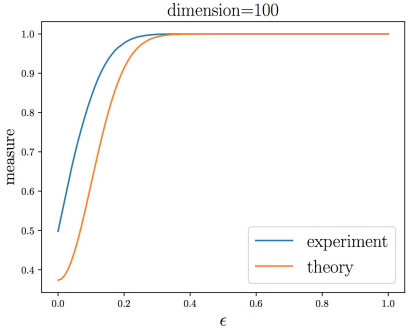


Figure: Understanding the robustness of a classifier in high-dimensional spaces. Shafahi et al. 2019.

Towards adversarial training for robustness

Adversarial Training

Let $h_{\mathbf{x}} : \mathbb{R}^n \to \mathbb{R}$ be a model with parameters $\mathbf{x}$ and let $\{(\mathbf{a}_i, \mathbf{b}_i)\}_{i=1}^n$, with the data $\mathbf{a}_i \in \mathbb{R}^p$ and the labels $\mathbf{b}_i$. The problem of adversarial training is the following adversarial optimization problem

$$\min_{\mathbf{x}} \frac{1}{n} \sum_{i=1}^{n} \left[\max_{\boldsymbol{\eta}:\|\boldsymbol{\eta}\| \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\eta}), \mathbf{b}_i) \right] \approx \min_{\mathbf{x}} \mathbb{E}_{(\mathbf{a},\mathbf{b})\sim\mathbb{P}} \left[\max_{\boldsymbol{\eta}:\|\boldsymbol{\eta}\| \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\eta}), \mathbf{b}_i) \right].$$

This problem can be formulated within the template $\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y})$.

Solving the outer problem

Adversarial Training

Let $h_{\mathbf{x}} : \mathbb{R}^n \to \mathbb{R}$ be a model with parameters $\mathbf{x}$ and let $\{(\mathbf{a}_i, \mathbf{b}_i)\}_{i=1}^n$, with $\mathbf{a}_i \in \mathbb{R}^p$ and $\mathbf{b}_i$ be the corresponding labels. The adversarial training optimization problem is given by

$$\min_{\mathbf{x}} \left\{ \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^{n} \underbrace{\left[\max_{\boldsymbol{\eta}: \|\boldsymbol{\eta}\| \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\eta}), \mathbf{b}_i) \right]}_{=: f_i(\mathbf{x})} \right\}.$$

Note that L is not continuously differentiable due to ReLU, max-pooling, etc.

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Note that L is not continuously differentiable due to ReLU, max-pooling, etc.

Question

How can we compute the gradient

$$\nabla_{\mathbf{x}} f_i(\mathbf{x}) := \nabla_{\mathbf{x}} \left(\max_{\boldsymbol{\eta}:\|\boldsymbol{\eta}\| \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\eta}), \mathbf{b}_i) \right)?$$

- **Challenge:** It involves differentiating with respect to a maximization.
- **A solution:** We can use Danskin's theorem under some conditions. See EPFL EE-556 (Lectures 9-10).

Basic first-order methods: GD and SGD

- Consider the finite sum (e.g., ERM) setting

$$f^\star := \min_{\mathbf{x}\in\mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{n}\sum_{j=1}^{n} f_j(\mathbf{x}) \right\}.$$

- Goal: Find $x^\star$ such that $\nabla f(x^\star) = 0$.

Algorithms in the finite sum setting

Gradient Descent	**Stochastic Gradient Descent**
$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k)$	$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k G(\mathbf{x}^k, \theta_k)$
$\nabla f(\mathbf{x}^k) = \frac{1}{n}\sum_{j=1}^{n} \nabla f_j(\mathbf{x}^k)$	$G(\mathbf{x}^k, \theta_k) = \nabla f_j(\mathbf{x}^k)$, $j \sim \text{Uniform}(\{1, \cdots, n\})$
α_k can be constant	$\mathbb{E}[G(\mathbf{x}^k, \theta_k)] = \nabla f(\mathbf{x}^k)$

- We will mostly focus on SGD in the sequel due to its scalability and generalization performance.

Stochastic Gradient Descent (SGD) and some key variants

Vanilla (Minibatch) SGD
Input: Stochastic gradient oracle $\mathbf{g}$, initial point $\mathbf{x}^0$, step size α_k
1. For $k = 0, 1, \ldots$:   obtain the (minibatch) stochastic gradient $\mathbf{g}^k$ update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \alpha_k \mathbf{g}^k$

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Perturbed Stochastic Gradient Descent [7]
Input: Stochastic gradient oracle $\mathbf{g}$, initial point $\mathbf{x}^0$, step size α_k
1. For $k = 0, 1, \ldots$:   sample noise ξ uniformly from unit sphere   update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \alpha_k(\mathbf{g}^k + \xi)$

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Stochastic Gradient Langevin Dynamics [25]

Input: Stochastic gradient oracle g, initial point $\mathbf{x}^0$, step size α_k

1. For $k = 0, 1, \ldots$

sample noise ξ standard Gaussian

update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \alpha_k \mathbf{g}^k + \sqrt{2\alpha_k}\xi$

Basic questions:

1. Does SGD converge with probability 1?
2. Does SGD avoid non-minimum points with probability 1?
3. How fast does SGD converge to local minimizers?

Critical points

Recall (Classification of critical points)

Let $f : \mathbb{R}^p \to \mathbb{R}$ be twice differentiable and let $\bar{\mathbf{x}}$ be a critical point, i.e., $\nabla f(\bar{\mathbf{x}}) = 0$. Let $\{\lambda_i\}_{i=1}^d$ be the eigenvalues of the hessian $\nabla^2 f(\bar{\mathbf{x}})$, then

- $\lambda_i > 0$ for all $i \Rightarrow \bar{\mathbf{x}}$ is a local minimum
- $\lambda_i < 0$ for all $i \Rightarrow \bar{\mathbf{x}}$ is a local maximum
- $\lambda_i > 0$, $\lambda_j < 0$ for some i, j and $\lambda_i \neq 0$ for all $i \Rightarrow \bar{\mathbf{x}}$ is a saddle point
- Other cases $\Rightarrow$ inconclusive

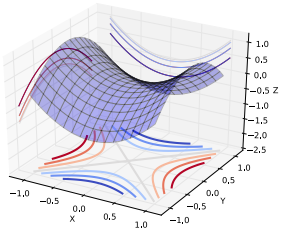


Figure: Minmax saddle ($\lambda_i \neq 0$ for all i)

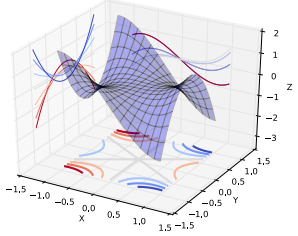


Figure: Monkey saddle ($\lambda_i = 0$ for some i)

Q1: Does SGD converge?

∘ SGD converges to the critical points of f as $k \to \infty$.

1. GD converges from any intialization with constant step-size and full gradients
2. With probability 1, (P)SGD does not converge with constant step-size α [2, 23]
3. With probability 1, SGD converges with vanishing step-size if $\mathbf{x}^k$ is bounded with probability 1 [16, 2]

Boundedness is not required (Theorem 1 of [18])

Assume Lipschitzness, sublevel regularity, $\mathbb{E}\|\mathbf{g}\|^q \leq \sigma^q$ and $\sum_k \alpha_k^{1+q/2} < \infty$ ($q \geq 2$). Then, $\mathbf{x}^k$ converges with probability 1.

Q2: Does SGD avoid saddle points?

- SGD avoids strict saddles ($\lambda_{\min}(\nabla^2 f(\bar{\mathbf{x}})) < 0$)

1. GD avoids strict saddles from almost all initializations [14]
2. With probability $1-\zeta$, PSGD with constant α escapes strict saddles after $\Omega\left(\log(1/\zeta)/\alpha^2\right)$ iterations [8]
   - However, SGD does not converge with constant α
   - We cannot take $\zeta = 0$

SGD avoids traps almost surely (Theorem 3 of [18])

Assume bounded uniformly exciting noise and $\alpha_k = \mathcal{O}\left(\frac{1}{k^\kappa}\right)$ for $\kappa \in (0, 1]$. Then, SGD avoids strict saddles from any initial condition with probability 1.

Q3: How fast does SGD converge to local minimizers?

- SGD remains close to Hurwicz minimizers (i.e., $\mathbf{x}^* : \lambda_{\min}(\nabla^2 f(\mathbf{x}^*)) > 0$)

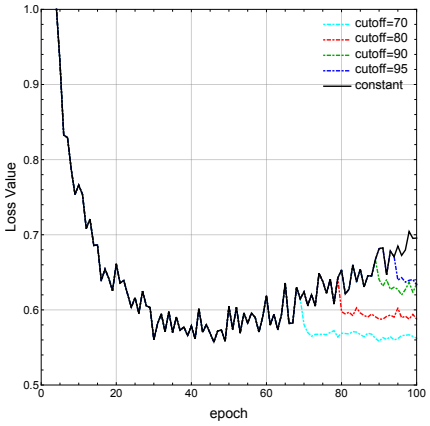
1. SGD with constant α can obtain objective value ϵ-close to a Hurwicz minimizer in $\mathcal{O}(1/\epsilon^2)$-iterations [8, 9]
   - However, SGD does not converge with constant α
   - Need averaging which is problematic in non-convex optimization

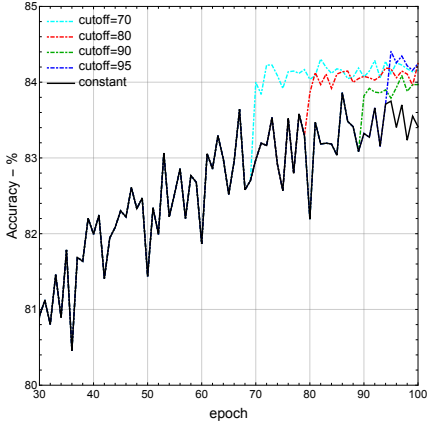
Using a vanishing step-size helps! (Theorem 4 of [18])

Using $\alpha_k = \mathcal{O}\left(\frac{1}{k}\right)$, SGD enjoys a $\mathcal{O}\left(\frac{1}{k}\right)$ convergence rate in objective value.

Using $1/k$ step-size decrease helps in practice

- ResNet training at different cool-down cut-offs





Worst-case iteration complexities of classical projected first-order methods[1][2]

$f(\mathbf{x})$	gradient oracle	L-smooth	Stationarity measure	GD/SGD	Accelerated GD/SGD
Convex	stochastic	yes	$f(\mathbf{x}^k) - f^\star =$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$
Convex	deterministic	yes	$f(\mathbf{x}^k) - f^\star =$	$\mathcal{O}\left(\frac{1}{k}\right)$	$\mathcal{O}\left(\frac{1}{k^2}\right)$
Convex	stochastic	no	$f(\mathbf{x}^k) - f^\star =$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$
Nonconvex	stochastic	yes	$\|G_\alpha(\mathbf{x}^k)\|^2 =$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^3$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^3$
Nonconvex	deterministic	yes	$\|G_\alpha(\mathbf{x}^k)\|^2 =$	$\mathcal{O}\left(\frac{1}{k}\right)^4$	$\mathcal{O}\left(\frac{1}{k}\right)^4$
Nonconvex	stochastic	no	$\mathrm{dist}(0, \partial(f(\mathbf{x}^k) + \delta_{\mathcal{X}}(\mathbf{x}^k)))^2 =$	?[3][5][6]	?[3][5][6]

- Basic structures, such as smoothness or strong convexity, help, but there are more structures that can be used:
  - $\max$-form, metric subregularity, Polyak-Łojasiewicz, Kurdyka-Łojasiewicz, weak convexity,[3] growth cond...

[1] Y. Nesterov, "Introductory lectures on convex optimization: A basic course," Springer Science, 2013.

[2] Y. Carmon, J.C. Duchi, O. Hinder, and A. Sidford, "Lower bounds for finding stationary points I–II." Mathematical Programming, 2019.

[3] D. Davis and D. Drusvyatskiy, "Stochastic model-based minimization of weakly convex functions," SIOPT, 2019.

[4] S. Ghadimi and G. Lan, "Accelerated gradient methods for nonconvex nonlinear and stochastic programming," MathProg, 2016.

[5] J. Zhang, et al., "On complexity of finding stationary points of nonsmooth nonconvex functions," arXiv:2002.04130, 2020.

[6] O. Shamir, "Can We Find Near-Approximately-Stationary Points of Nonsmooth Nonconvex Functions?" arXiv:2002.11962, 2020.

Detour: Weak convexity (WeCo) & approximate stationarity[1]

- Smooth: Gradient mapping norm
  - $\|G_\alpha(\mathbf{x}^k)\|^2 = \frac{1}{\alpha^2}\|x^k - \pi_{\mathcal{X}}(\mathbf{x}^k - \alpha\nabla f(\mathbf{x}^k))\|^2$
  - possible to compute
- Non-smooth: Generalized subdifferential distance
  - $\text{dist}(0, \partial(f(\mathbf{x}^k) + \delta_{\mathcal{X}}(\mathbf{x}^k)))^2$
  - hard in general (even approximately)[2][3]

- f is ρ-weakly convex if $f(\mathbf{x}) + \frac{\rho}{2}\|\mathbf{x}\|^2$ is convex.

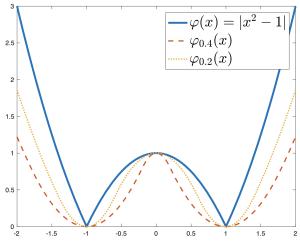


Figure: ME with $f(x) = |x^2 - 1|$, $\mathcal{X} = \mathbb{R}$, and $\hat{v}_t = \mathbb{I}$.[1]

- Moreau envelope (ME):

$$\varphi_{1/\rho}(\mathbf{x}) = \min_{y\in\mathcal{X}} \left\{ f(\mathbf{y}) + \frac{\rho}{2}\|\mathbf{y} - \mathbf{x}\|^2 \right\}$$

$$\hat{\mathbf{x}} \leftarrow \arg\min$$

$$\nabla\varphi_{1/\rho}(x) = \rho(\mathbf{x} - \hat{\mathbf{x}})$$

- Small $\|\nabla\phi_{1/\rho}(\mathbf{x})\|$ implies near-stationarity:[1]

$$\text{dist}(0, \partial(f(\mathbf{x}^k) + \delta_{\mathcal{X}}(\mathbf{x}^k)))^2 \leq \|\nabla\phi_{1/\rho}(\mathbf{x}^k)\|^2$$

  - also implies small $\|G_\alpha(\mathbf{x}^k)\|^2$ if f is smooth

[1] D. Davis and D. Drusvyatskiy, "Stochastic model-based minimization of weakly convex functions," SIOPT, 2019.
[2] J. Zhang, et al., "On complexity of finding stationary points of nonsmooth nonconvex functions," arXiv:2002.04130, 2020.
[3] O. Shamir, "Can We Find Near-Approximately-Stationary Points of Nonsmooth Nonconvex Functions?" arXiv:2002.11962, 2020.

A comparison of adaptive algorithms

	GD/SGD	Accelerated GD/SGD	AdaGrad	AcceleGrad/UniXgrad	Adam/AMSGrad
Convex, stochastic	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^2$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^2$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^3$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^{4,5}$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^6$
Convex, deterministic, L-smooth	$\mathcal{O}\left(\frac{1}{k}\right)^2$	$\mathcal{O}\left(\frac{1}{k^2}\right)^2$	$\mathcal{O}\left(\frac{1}{k}\right)^4$	$\mathcal{O}\left(\frac{1}{k^2}\right)^{4,5}$	$\mathcal{O}\left(\frac{1}{k}\right)^7$
Nonconvex, stochastic, L-smooth	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^2$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^2$	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^8$	?	$\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)^9$
Nonconvex, deterministic, L-smooth	$\mathcal{O}\left(\frac{1}{k}\right)^2$	$\mathcal{O}\left(\frac{1}{k}\right)^2$	$\mathcal{O}\left(\frac{1}{k}\right)^8$	?	$\mathcal{O}\left(\frac{1}{k}\right)^7$

[2] Lan, First-order and Stochastic Optimization Methods for Machine Learning. Springer Nature, 2020.

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Chen, Zhou, Tang, Yang, Cao, Gu, Closing the generalization gap of adaptive gradient methods in training deep neural networks, IJCAI 2020.
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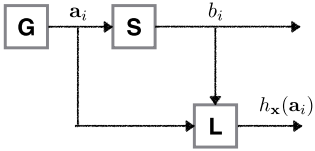
From empirical risk minimization...



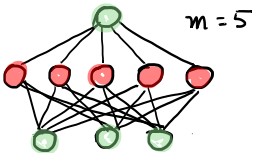
Definition (Optimization formulation)

The deep-learning training problem is given by

$$\mathbf{x}^\star_{\mathsf{DL}} \in \arg\min_{\mathbf{x}\in\mathcal{X}} \{\, f(\mathbf{x}) := \frac{1}{n}\sum_{i=1}^{n} L(h_{\mathbf{x}}(\mathbf{a}_i), b_i) \,\},$$

where $\mathcal{X}$ denotes the constraints on the parameters.

- A single hidden layer neural network with params $\mathbf{x} := [\mathbf{X}_1, \mathbf{X}_2, \mu_1, \mu_2]$



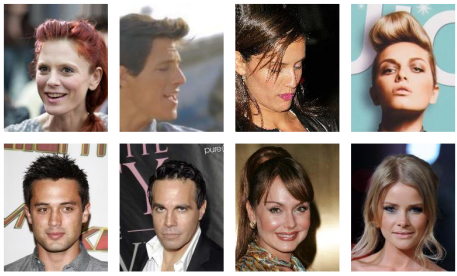
$$h_{\mathbf{x}}(\mathbf{a}) := \begin{bmatrix} \mathbf{X}_2 \end{bmatrix} \sigma \left(\begin{bmatrix} \mathbf{X}_1 \end{bmatrix} \begin{bmatrix} \mathbf{a} \end{bmatrix} + \begin{bmatrix} \mu_1 \end{bmatrix} \right) + \begin{bmatrix} \mu_2 \end{bmatrix}$$

activation (over σ); weight (over $\mathbf{X}_1$); input (over $\mathbf{a}$); bias (over μ_1); bias (over μ_2)

hidden layer = learned features

Into generative adversarial networks (GANs)

- Key parametric density estimation setting

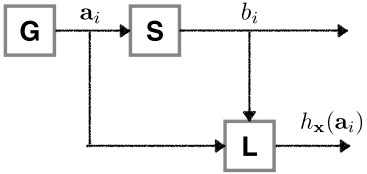


(source: http://mmlab.ie.cuhk.edu.hk/projects/CelebA.html)

$\mathbf{a}_i = [$ ...images...$]$

$b_i = [$ ...probability... $]$

- Goal: Games, denoising, image recovery...



- Generator $\mathbb{P}_{\mathbf{a}}$
  - Nature
- Supervisor $\mathbb{P}_{B|\mathbf{a}}$
  - Frequency data
- Learning Machine $h_{\mathbf{x}}(\mathbf{a}_i)$
  - Data scientist: Mathematics of Data

A way to model complex distributions: The push-forward measure

- Traditionally, we use analytical distributions: Restricts what we could model in real applications.
- Now, we use more expressive probability measures via *push-forward measures* with neural networks.

Definition

- Let $\omega \sim \mathrm{p}_\Omega$ be a random variable.
- $h_{\mathbf{x}}(\cdot) : \mathbb{R}^p \to \mathbb{R}^m$ a function parameterized by parameters $\mathbf{x}$.

The pushforward measure of p_Ω under $h_{\mathbf{x}}$, denoted by $h_{\mathbf{x}} \# \mathrm{p}_\Omega$ is the distribution of $h_{\mathbf{x}}(\omega)$.

Towards an optimization problem

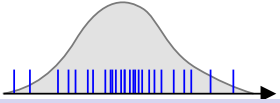
Problem (Ideal parametric density estimator)

Given a true distribution $\mu^\natural$, we can solve the following optimization problem,

$$\min_{\mathbf{x}} W_1(\mu^\natural, h_{\mathbf{x}} \# \mathsf{p}_\Omega), \tag{1}$$

where the measurable function $h_{\mathbf{x}}$ is parameterized by $\mathbf{x}$ and $\omega \sim \mathsf{p}_\Omega$ is "simple."

- We can minimize $W_1\left(\hat{\mu}_n, h_{\mathbf{x}} \# \mathsf{p}_\Omega\right)$ with respect to $\mathbf{x}$.
- Figure: Empirical distribution (blue), $\hat{\mu}_n = \sum_{i=1}^n \delta_i$



A plug-in empirical estimator

Using the triangle inequality for Wasserstein distances we can upper bound in the follow way,

$$W_1(\mu^\natural, h_{\mathbf{x}} \# \mathsf{p}_\Omega) \leq W_1(\mu^\natural, \hat{\mu}_n) + W_1(\hat{\mu}_n, h_{\mathbf{x}} \# \mathsf{p}_\Omega), \tag{2}$$

where $\hat{\mu}_n$ is the empirical estimator of $\mu^\natural$ obtained from n independent samples from $\mu^\natural$.

Remarks:

- Using an empirical estimator in high-dimensions is terrible in the worst case [24, 6].
- However, it does not directly say that $W_1\left(\mu^\natural, h_{\mathbf{x}} \# \mathsf{p}_\Omega\right)$ will be large.

Duality of 1-Wasserstein: Towards a minimax formulation

Theorem (Kantorovich-Rubinstein duality)

$$W_1(\mu, \nu) = \sup_{\mathtt{d}} \{\langle \mathtt{d}, \mu \rangle - \langle \mathtt{d}, \nu \rangle : \mathtt{d} \textit{ is 1-Lipschitz}\} \tag{3}$$

Remark: ○ $\mathtt{d}$ is the "dual" variable. In the literature, it is commonly referred to as the "discriminator."

Inner product is an expectation

$$\langle \mathtt{d}, \mu \rangle = \int \mathtt{d} \mathrm{d}\mu = \int \mathtt{d}(\mathbf{a}) \mathrm{d}\mu(\mathbf{a}) = \boldsymbol{E}_{\mathbf{a} \sim \mu} \left[\mathtt{d}(\mathbf{a}) \right]. \tag{4}$$

Kantorovich-Rubinstein duality applied to our objective

$$W_1\left(\hat{\mu}_n, h_{\mathbf{x}} \# \omega\right) = \sup_{\mathtt{d}} \left\{ \boldsymbol{E}_{\mathbf{a} \sim \hat{\mu}_n} [\mathtt{d}(\mathbf{a})] - \boldsymbol{E}_{\mathbf{a} \sim h_{\mathbf{x}} \# \omega} [\mathtt{d}(\mathbf{a})] : \mathtt{d} \text{ is 1-Lipschitz} \right\} \tag{5}$$

Wasserstein GANs formulation

- Ingredients:
  - fixed *noise* distribution p_Ω (e.g., normal)
  - target distribution $\hat{\mu}_n$ (natural images)
  - $\mathcal{X}$ parameter class inducing a class of functions (generators)
  - $\mathcal{Y}$ parameter class inducing a class of functions (dual variables)

Wasserstein GANs formulation [1]

Define a parameterized function $\mathsf{d}_{\mathbf{y}}(\mathbf{a})$, where $\mathbf{y} \in \mathcal{Y}$ such that $\mathsf{d}_{\mathbf{y}}(\mathbf{a})$ is 1-Lipschitz. In this case, the Wasserstein GAN optimization problem is given by

$$\min_{\mathbf{x}\in\mathcal{X}} \left(\max_{\mathbf{y}\in\mathcal{Y}} \boldsymbol{E}_{\mathbf{a}\sim\hat{\mu}_n} \left[\mathsf{d}_{\mathbf{y}}(\mathbf{a})\right] - \boldsymbol{E}_{\boldsymbol{\omega}\sim\mathsf{p}_\Omega} \left[\mathsf{d}_{\mathbf{y}}(h_{\mathbf{x}}(\boldsymbol{\omega}))\right] \right). \tag{6}$$

This problem can be formulated within the template $\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y})$.

Remarks:
- Cannot solve in a manner similar to adversarial training a la Danskin. Need a direct approach.
- Scalability, model collapse, catastrophic forgetting. Heuristics galore!
- Enforce Lipschitz constraint weight clipping, gradient penalty, spectral normalization [1, 10, 19].

Abstract minmax formulation

Minimax formulation

$$\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y}), \tag{7}$$

where

- Φ is differentiable and nonconvex in $\mathbf{x}$ and nonconcave in $\mathbf{y}$,
- The domain is unconstrained, specifically $\mathcal{X}=\mathbb{R}^m$ and $\mathcal{Y}=\mathbb{R}^n$.

- Key questions:

1. Where do the algorithms converge?
2. When do the algorithm converge?

Abstract minmax formulation

Minimax formulation

$$\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y}), \tag{7}$$

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- Φ is differentiable and nonconvex in $\mathbf{x}$ and nonconcave in $\mathbf{y}$,
- The domain is unconstrained, specifically $\mathcal{X} = \mathbb{R}^m$ and $\mathcal{Y} = \mathbb{R}^n$.

○ Key questions:

1. Where do the algorithms converge?
2. When do the algorithm converge?

A buffet of negative results [5]

"Even when the objective is a Lipschitz and smooth differentiable function, deciding whether a min-max point exists, in fact even deciding whether an approximate min-max point exists, is NP-hard. More importantly, an approximate local min-max point of large enough approximation is guaranteed to exist, but finding one such point is PPAD-complete. The same is true of computing an approximate fixed point of the (Projected) Gradient Descent/Ascent update dynamics."

Solution concept

- Like for nonconvex problems in minimization we try to find a *local* solution.

Definition (Local Nash Equilibrium)

A pure strategy $(\mathbf{x}^\star, \mathbf{y}^\star)$ is called a Local Nash Equilibrium (LNE) if,

$$\Phi\left(\mathbf{x}^\star, \mathbf{y}\right) \leq \Phi\left(\mathbf{x}^\star, \mathbf{y}^\star\right) \leq \Phi\left(\mathbf{x}, \mathbf{y}^\star\right) \tag{LNE}$$

for all $\mathbf{x}$ and $\mathbf{y}$ within some neighborhood of $\mathbf{x}^\star$ and $\mathbf{y}^\star$, i.e., $\|\mathbf{x} - \mathbf{x}^\star\| \leq \delta$ and $\|\mathbf{y} - \mathbf{y}^\star\| \leq \delta$ for some $\delta > 0$.

Necessary conditions

Through a Taylor expansion around $\mathbf{x}^\star$ and $\mathbf{y}^\star$ one can show that a LNE implies,

$$\nabla_{\mathbf{x}} \Phi(\mathbf{x}, \mathbf{y}), -\nabla_{\mathbf{y}} \Phi(\mathbf{x}, \mathbf{y}) = 0$$
$$\nabla_{\mathbf{xx}} \Phi(\mathbf{x}, \mathbf{y}), -\nabla_{\mathbf{yy}} \Phi(\mathbf{x}, \mathbf{y}) \succeq 0$$

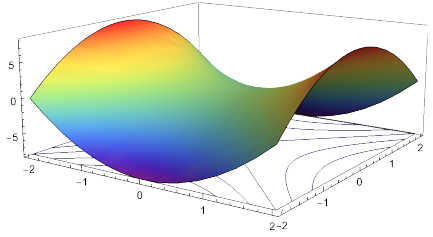

Figure: $\Phi(x, y) = x^2 - y^2$

Recall SGD results

$$\min_{\mathbf{x}:\mathbf{x}\in\mathcal{X}} f(\mathbf{x})$$

- For a non-convex, smooth f, we have that

1. SGD converges to the critical points of f as $N \to \infty$.
2. SGD avoids strict saddles/traps ($\lambda_{\min}(\nabla^2 f(\mathbf{x}^*)) < 0$) almost surely.
3. SGD remains close to Hurwicz minimizers (i.e., $\mathbf{x}^* : \lambda_{\min}(\nabla^2 f(\mathbf{x}^*)) > 0$ almost surely.

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- Nail in the coffin:
  - not even sure if we obtain stochastic descent directions by approximately solving inner problems in GANs.
  - GANs are fundamentally different from adversarial training!
- Need more direct approaches with the stochastic gradient estimates.

Basic algorithms for minimax

- Given $\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y})$, define $V(\mathbf{z}) = [-\nabla_{\mathbf{x}}\Phi(\mathbf{x},\mathbf{y}), \nabla_{\mathbf{y}}\Phi(\mathbf{x},\mathbf{y})]$ with $\mathbf{z} = [\mathbf{x},\mathbf{y}]$.

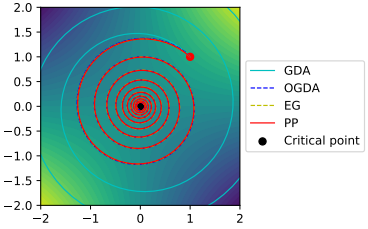

Figure: Trajectory of different algorithms for a simple bilinear game $\min_x \max_y xy$.

- (In)Famous algorithms
  - Gradient Descent Ascent (GDA)
  - Proximal point method (PPM)
  - Extra-gradient (EG)
  - Optimistic Gradient Descent Ascent (OGDA)
  - Reflected-Forward-Backward-Splitting (RFBS)

- EG and OGDA are approximations of the PPM
  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha\mathbf{V}(\mathbf{z}^k)$.
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  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha\mathbf{V}(\mathbf{z}^k - \alpha\mathbf{V}(\mathbf{z}^{k-1}))$
  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha[2\mathbf{V}(\mathbf{z}^k) - \mathbf{V}(\mathbf{z}^{k-1})]$
  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha\mathbf{V}(2\mathbf{z}^k - \mathbf{z}^{k-1})$

Generalized Robbins-Monro schemes

- Given $\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y})$, define $V(\mathbf{z}) = [-\nabla_{\mathbf{x}}\Phi(\mathbf{x},\mathbf{y}), \nabla_{\mathbf{y}}\Phi(\mathbf{x},\mathbf{y})]$ with $\mathbf{z} = [\mathbf{x},\mathbf{y}]$.
- Given $V(\mathbf{z})$, define stochastic estimates of $V(\mathbf{z},\zeta) = V(\mathbf{z}) + U(\mathbf{z},\zeta)$, where
  - $U(\mathbf{z},\zeta)$ is a bias term
  - We often have unbiasedness: $\boldsymbol{E}U(\mathbf{z},\zeta) = 0$
  - The bias term can have bounded moments
  - We often have bounded variance: $P(\|U(\mathbf{z},\zeta)\| \geq t) \leq 2\exp -\frac{t^2}{2\sigma^2}$ for $\sigma > 0$.
- An abstract template for generalized Robbins-Monro schemes, dubbed as $\mathcal{A}$:

$$\mathbf{z}^{k+1} = \mathbf{z}^k + \alpha_k V(\mathbf{z}^k, \zeta^k)$$

The dessert section in the buffet of negative results: [12]

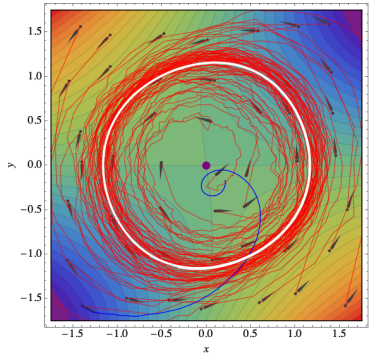
1. Bounded trajectories of $\mathcal{A}$ always converge to an internally chain-transitive (ICT) set.
2. Trajectories of $\mathcal{A}$ may converge with arbitrarily high probability to spurious attractors that contain no critical point of Φ.

Minimax is more difficult than just optimization [12]

- Internally chain-transitive (ICT) sets characterize the convergence of dynamical systems [3].
  - For optimization, {attracting ICT} $\equiv$ {solutions}
  - For minimax, {attracting ICT} $\equiv$ {solutions} $\cup$ {spurious sets}

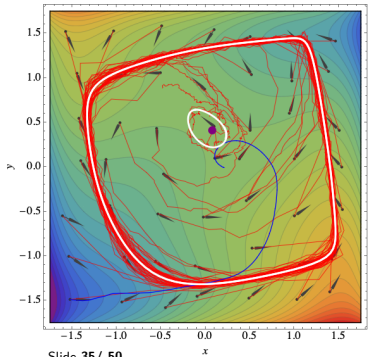
- "Almost" bilinear $\neq$ bilinear:

$$\Phi(x,y) = xy + \epsilon\phi(x), \phi(x) = \frac{1}{2}x^2 - \frac{1}{4}x^4$$



- The "forsaken" solutions:

$$\Phi(y,x) = y(x-0.5)+\phi(y)-\phi(x), \phi(u) = \frac{1}{4}u^2-\frac{1}{2}u^4+\frac{1}{6}u^6$$



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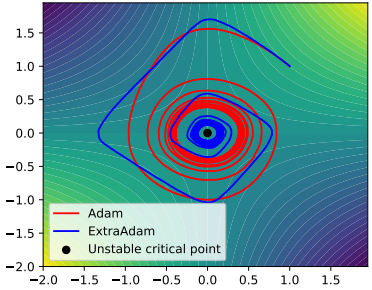

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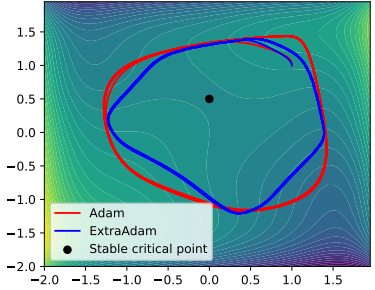


A summary of results for nonconvex-concave setting

- A summary of gradient complexities to reach $\epsilon-$first order stationary point in terms of **gradient mapping.**

Method	Assumption on $\Phi(\cdot,\cdot)$	Convergence rate	Reference
GDA	noconvex-concave	$\tilde{\mathcal{O}}\left(\epsilon^{-6}\right)$	[15]
GDA	nonconvex- strongly concave	$\mathcal{O}\left(\epsilon^{-2}\right)$	[15]
GDmax	nonconvex-concave	$\tilde{\mathcal{O}}\left(\epsilon^{-6}\right)$	[13]
GDmax	nonconvex- strongly concave	$\mathcal{O}\left(\epsilon^{-2}\right)$	[13]
HiBSA, AGP	nonconvex-concave	$\tilde{\mathcal{O}}\left(\epsilon^{-4}\right)$	[17], [26]
HiBSA, AGP	nonconvex- strongly concave	$\mathcal{O}\left(\epsilon^{-2}\right)$	[17], [26]

Comparison of convergence rates for smooth convex-concave minimax

Method	Assumption on $\Phi(\cdot,\cdot)$	Convergence rate	Reference	Note
PP	convex-concave	$\mathcal{O}\left(\epsilon^{-1}\right)$	[22]	
PP	strongly convex- strongly concave	$\mathcal{O}\left(\kappa \log(\epsilon^{-1})\right)$	[22]	Implicit algorithm
PP	Bilinear	$\mathcal{O}\left(\kappa \log(\epsilon^{-1})\right)$	[22]	
EG	convex-concave	$\mathcal{O}\left(\epsilon^{-1}\right)$	[20]	
EG	strongly convex- strongly concave	$\mathcal{O}\left(\kappa \log(\epsilon^{-1})\right)$	[21, 20]	1 extra-gradient evaluation per iteration
EG	Bilinear	$\mathcal{O}\left(\kappa \log(\epsilon^{-1})\right)$	[21, 20]	
OGDA	convex-concave	$\mathcal{O}\left(\epsilon^{-1}\right)$	[20]	
OGDA	strongly convex- strongly concave	$\mathcal{O}\left(\kappa \log(\epsilon^{-1})\right)$	[21, 20]	no obvious downside
OGDA	Bilinear	$\mathcal{O}\left(\kappa \log(\epsilon^{-1})\right)$	[21, 20]	

Lifting minimax optimization: From pure to mixed Nash equilibrium

- Rethinking minimax problem as pure strategy game formulation

$$\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y})$$

- A corresponding **mixed** strategy formulation

$$\min_{p\in\mathcal{M}(\mathcal{X})} \max_{q\in\mathcal{M}(\mathcal{Y})} \mathbb{E}_{\mathbf{x}\sim p}\mathbb{E}_{\mathbf{y}\sim q}\left[\Phi(\mathbf{x},\mathbf{y})\right]$$

  - $\mathcal{M}(\mathcal{Z}) \coloneqq \{\text{all randomized strategies on } \mathcal{Z}\}$
  - There is a way to solve this infinite dimensional problem: Mirror descent + Langevin dynamics [11]

From pure to mixed Nash equilibrium

- Key ingredients
  - $\langle p, h \rangle \coloneqq \int h \, \mathrm{d}p$ for a measure p and function h (Riesz representation)
  - the linear operator G and its adjoint $G^\dagger$:

$$\begin{aligned} (Gq)(\mathbf{x}) &\coloneqq \mathbb{E}_{\mathbf{y}\sim q}\left[\Phi(\mathbf{x},\mathbf{y})\right] \\ (G^\dagger p)(\mathbf{y}) &\coloneqq \mathbb{E}_{\mathbf{x}\sim p}\left[\Phi(\mathbf{x},\mathbf{y})\right], \end{aligned}$$

- Mixed NE formulation $\simeq$ finite two-player games

$$\min_{p\in\mathcal{M}(\mathcal{X})} \max_{q\in\mathcal{M}(\mathcal{Y})} \mathbb{E}_{\mathbf{x}\sim p}\mathbb{E}_{\mathbf{y}\sim q}\left[\Phi(\mathbf{x},\mathbf{y})\right]$$

$$\Updownarrow$$

$$\min_{p\in\mathcal{M}(\mathcal{X})} \max_{q\in\mathcal{M}(\mathcal{Y})} \langle p, Gq \rangle$$

  - If $\mathcal{X}$ and $\mathcal{Y}$ are finite $\Rightarrow$ mirror descent
  - Caveat: **infinite dimension!!!** See solution details in [11].

Application: Noisy action robust reinforcement learning[1]

- Train RL agent in the presence of an adversary
- Adversary budget: $\alpha \in [0, 0.5]$

Noisy action robust MDP game

for $t = 1, 2, \ldots$ do:

both players observe state $S_t \in \mathcal{S}$

both players choose actions $A_t = \mu(S_t) \in \mathcal{A}$, and $A'_t = \nu(S_t) \in \mathcal{A}$

execute the noisy action $\bar{A}_t = (1 - \alpha)A_t + \alpha A'_t$

agent gets reward $R_{t+1} = R(S_t, \bar{A}_t)$, adversary gets $-R_{t+1}$

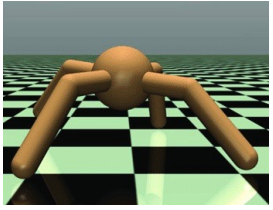
both players enter new state S_{t+1}

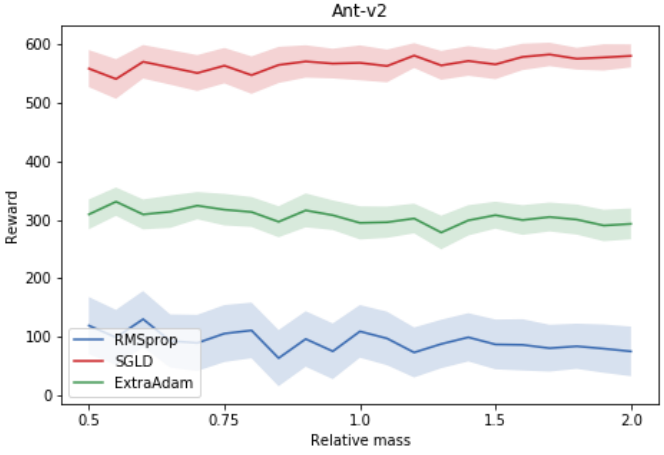
- Hope: Train in one environment, generalize to others

[1] K. Parameswaran, Y-T. Huang, Y-P. Hsieh, P. Rolland, C. Shi, and V. Cevher, "Robust Reinforcement Learning via Adversarial training with Langevin Dynamics" In NeurIPS, 2020.

Experimental evaluation via MuJoCo

- Standard MuJoCo datasets





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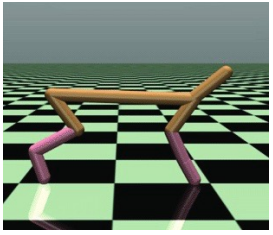
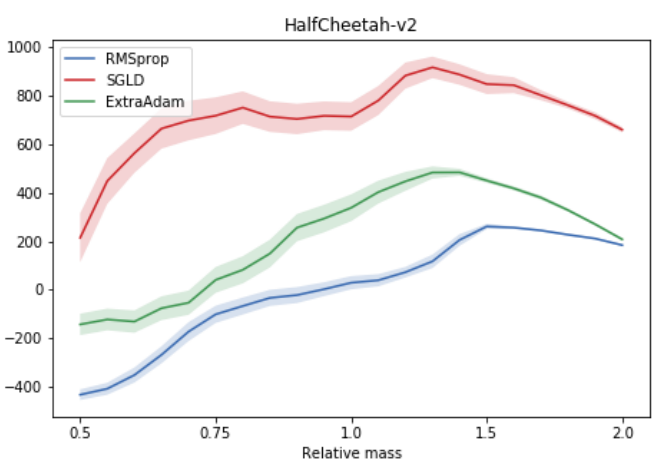
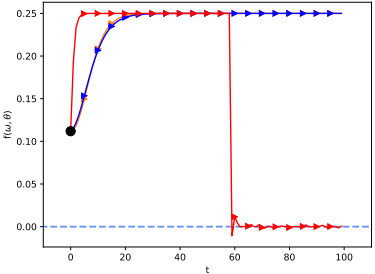
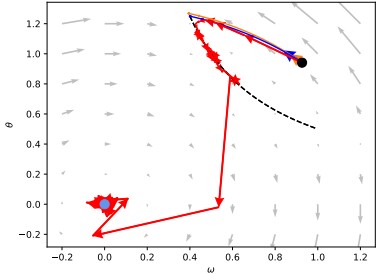


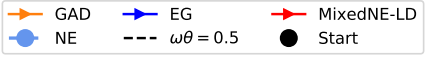


Escaping traps with the mixed-NE concept

$$\max_{\omega\in[-2,2]} \min_{\theta\in[-2,2]} -\omega^2\theta^2 + \omega\theta$$







Thank you for your attention![10]

- Minimax is more difficult than just optimization!
- It is possible to avoid limit cycles under right settings (upcoming work!)
- Universal adaptation is an open research topic

[10] Postdoc positions are available in my group!

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