## Instability, Computational Efficiency, and Statistical Accuracy

#### Nhat Ho

#### University of Texas, Austin

Joint work with Raaz Dwivedi, Michael I. Jordan, Koulik Khamaru, Tongzheng Ren, Sujay Sanghavi, Purnamrita Sarkar, Martin J. Wainwright, Rachel Ward, Bin Yu

June, 2024

Nhat Ho (Univ of Texas, Austin)

June 2024 1 / 41

= 900

(3) (3) (4) (3)

# Talk outline

Challenges with optimization methods in statistical machine learning models

- Population to sample analysis framework
  - Contraction of population operator
  - Stability of sample operator
- 3 Convergence of optimization methods under different settings of operators
  - Stable and fast operators
  - Stable and slow operators
  - Unstable and fast operators
  - Unstable and slow operators

#### Optimality of exponentially increasing step size gradient descent

#### Main stories

- Unstable optimization algorithms can be preferred to stable ones
- Exponentially increasing step size can be computationally optimal for statistical estimation

## Parametric statistical machine learning models

• Given a random sample of size *n* 

$$X_1,\ldots,X_n \sim f_{\theta^\star}(x)$$

- Known: family of distributions  $\{f_{\theta}(x), \theta \in \Theta\}$
- Unknown:  $\theta^*$

(4) (3) (4) (4) (4)

## Estimation methods

- Standard approaches to estimate θ<sup>\*</sup> include M-estimators (e.g., least-square, MLE), methods of moments, etc.
- Challenge:  $f_{\theta}$  is generally non-convex function and optimal solutions from these approaches do not admit closed-forms
- Solution: Optimization algorithms are used to approximate  $\theta^*$

## Fundamental questions

- Under what conditions does an optimization algorithm achieve a statistically optimal rate?
- When is an unstable optimization algorithm, such as Newton's method, preferred to a stable algorithm, such as gradient descent method?
- Will increasing step size, instead of decreasing step size, be statistically and computationally optimal?

▲ 国 ▶ | ▲ 国 ▶

First example: Non-linear regression model

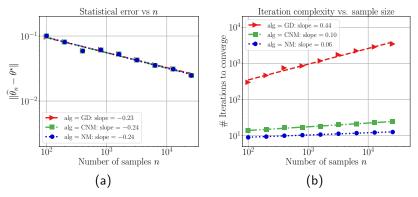
•  $\{(X_i,Y_i)\}_{i=1}^n$  are generated from a noisy non-linear regression model of the form

$$Y_i = g\left(X_i^{\top} \theta^{\star}\right) + \xi_i, \quad \text{for } i = 1, \dots, n.$$

- $\xi_i$  is a zero-mean noise variable with variance  $\sigma^2$
- $g(t) = t^2$  for  $t \in \mathbb{R}$

A B M A B M

## Behavior of optimization algorithms



The behavior of gradient descent (GD), cubic-regularized Newton's method (CNM), and the Newton's method (NM) for the regression model when  $\theta^* = 0$ .

- All the algorithms achieve optimal statistical rates  $n^{-1/4}$
- Newton's method takes least number of steps (≈ log(n)) while gradient descent takes significantly larger number of steps (≈ √n)

## Second example: Mixture model

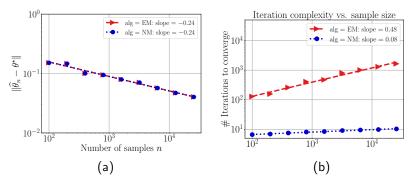
• Two-component Gaussian mixtures:

- True model:  $\frac{1}{2}\mathcal{N}(-\theta^{\star},\mathbb{I}_d) + \frac{1}{2}\mathcal{N}(\theta^{\star},\mathbb{I}_d)$
- Fitted model:  $\frac{1}{2}\mathcal{N}(-\theta,\mathbb{I}_d) + \frac{1}{2}\mathcal{N}(\theta,\mathbb{I}_d)$



(4) (3) (4) (4) (4)

## Behavior of optimization algorithms



The behavior of Expectation-Maximization (EM) algorithm and the Newton's method (NM) for the mixture model when  $\theta^{\star} = 0$ .

- EM and Newton's method achieve optimal statistical rates  $n^{-1/4}$
- Newton's method takes  $\approx \log(n)$  steps to converge while EM algorithm takes significantly larger number of steps ( $\approx \sqrt{n}$ )

## General framework

- $F_n$ : the empirical operator
  - ► Example:  $F_n(\theta) = \theta \eta \nabla f_n(\theta)$  where  $f_n$  is sample log-likelihood function
- F: the population operator
  - ► Example:  $F(\theta) = \theta \eta \nabla f(\theta)$  where f is population log-likelihood function, i.e., the limit of  $f_n$  when  $n \to \infty$
- $\theta^{\star}$ : fixed point of F, i.e.,  $F(\theta^{\star}) = \theta^{\star}$

• 
$$\theta_n^{t+1} = F_n(\theta_n^t)$$
 for  $t = 1, 2, ...$ 

#### Question

Under which conditions,  $\{\theta_n^t\}$  approaches a suitably defined neighborhood of  $\theta^*$ ?

## Population to sample analysis<sup>1</sup>

• Triangle inequality:

$$\|\theta_n^{t+1} - \theta^\star\| = \|F_n(\theta_n^t) - \theta^\star\| \le \underbrace{\|F(\theta_n^t) - \theta^\star\|}_A + \underbrace{\|F_n(\theta_n^t) - F(\theta_n^t)\|}_B$$

- A: Contraction of population operator
- B: Deviation between sample and population operators

<sup>1</sup>(Yi and Caramanis, 2015), (Hardt et al., 2016), (Balakrishnan et al., 2017), (Chen et al., 2018), (Kuzborskij and Lampert, 2018), (Charles and Papailiopoulos, 2018), (Dwivedi et al., 2020a,b), etc.

Nhat Ho (Univ of Texas, Austin)

### Contraction of population operator F

There are two types of contractions:

• Fast convergence: For  $\kappa \in (0,1)$ , F is FAST( $\kappa$ )-convergent if

 $\|F^t(\theta_0) - \theta^\star\| \le \kappa^t \|\theta_0 - \theta^\star\| \quad \text{for all } t = 1, 2, \dots$ 

• Slow convergence: For  $\beta > 0$ , F is SLOW( $\beta$ )-convergent if

$$\|F^t(\theta_0) - \theta^\star\| \le \frac{c}{t^{\beta}}$$
 for all  $t = 1, 2, \dots$ 

### Example: Fast versus slow convergence

We consider  $\min_{\theta} f(\theta) = \frac{\theta^{2p}}{2p}$  for some  $p \ge 1$ 

• Gradient descent algorithm:

$$F(\theta) = \theta - \eta \nabla f(\theta) = \theta \left( 1 - \eta \theta^{2p-2} \right)$$

• When p = 1, F is FAST( $\kappa$ )-convergent algorithm with  $\kappa = 1 - \eta$ 

• When  $p \ge 2$ , F is SLOW( $\beta$ )-convergent with  $\beta = \frac{1}{2p-2}$ 

(日本)

Deviation between sample and population operators

There are two types of deviations:

• Stability condition: For  $\gamma \geq 0$ ,  $F_n$  is STA( $\gamma$ )-stable with noise  $\varepsilon(\cdot)$  if

$$\mathbb{P}\Big[\sup_{\theta\in\mathsf{Ball}(\theta^{\star},r)}\|F_n(\theta)-F(\theta)\|\precsim \min\Big\{r^{\gamma}\varepsilon(n,\delta),r\Big\}\Big]\geq 1-\delta$$

for any r > 0

• Instability condition: For  $\gamma < 0$ ,  $F_n$  is UNS( $\gamma$ )-unstable with noise  $\varepsilon(\cdot)$  if

$$\mathbb{P}\left[\sup_{\theta\in\mathsf{Annulus}(\theta^{\star},r,\rho_{\mathrm{out}})}\|F_{n}(\theta)-F(\theta)\|\leq\varepsilon(n,\delta)\max\left\{\frac{1}{r^{|\gamma|}},\rho_{\mathrm{out}}\right\}\right]\geq1-\delta$$

for any radius  $r \ge \rho_{in}$ .

<sup>1</sup>Annulus( $\theta^*, r, \rho_{\text{out}}$ ) = { $\theta$  :  $r \le \|\theta - \theta^*\| \le \rho_{\text{out}}$ }

Nhat Ho (Univ of Texas, Austin)

### Example of stable condition

• 
$$\min_{\theta} f_n(\theta) = \frac{\theta^4}{4} + \frac{w}{2\sqrt{n}}\theta^2$$
 where  $w \sim N(0, \sigma^2)$ 

- Gradient descent:
  - ▶ Sample operator:  $F_n(\theta) = \theta \left(1 \eta \theta^2 \eta \frac{w}{\sqrt{n}}\right)$
  - Population operator:  $F(\theta) = \theta \left(1 \eta \theta^2\right)$
- With probability  $1 \delta$ ,

$$|F_n(\theta) - F(\theta)| = \eta |\theta| \frac{|w|}{\sqrt{n}} \precsim |\theta| \sqrt{\frac{\log(1/\delta)}{n}}$$

 $\implies F_n \text{ is STA}(\gamma) \text{-stable with } \gamma = 1 \text{ and noise } \varepsilon(n, \delta) = \sqrt{\log(1/\delta)/n}$ 

## Example of unstable condition

• 
$$\min_{\theta} f_n(\theta) = \frac{\theta^4}{4} + \frac{w}{2\sqrt{n}}\theta^2$$
 where  $w \sim N(0, \sigma^2)$ 

- Newton's method:
  - ► Sample operator:  $F_n(\theta) = \theta \frac{\theta^3 + w\theta/\sqrt{n}}{3\theta^2 + w/\sqrt{n}}$
  - Population operator:  $F(\theta) = \theta \frac{\theta^3}{3\theta^2}$
- With probability  $1 \delta$ , when  $|\theta| \succeq \left(\frac{\log(1/\delta)}{n}\right)^{1/4}$ :

$$|F_n(\theta) - F(\theta)| \precsim \frac{1}{|\theta|} \sqrt{\frac{\log(1/\delta)}{n}}$$

 $\Longrightarrow F_n$  is UNS( $\gamma$ )-unstable with parameter  $\gamma=-1$  and noise  $\varepsilon(n,\delta)=\sqrt{\log(1/\delta)/n}$ 

▲□ ▲ □ ▲ ■ ▲ ■ ■ ■ ● ● ●

## General theory: Stable and fast operators

- The operator F is FAST( $\kappa$ )-convergent
- The empirical operator  $F_n$  is STA( $\gamma)$ -stable with noise  $\varepsilon(n,\delta)$  for some  $\gamma \geq 0$

Theorem 1 (Balakrishnan et al., 2017<sup>2</sup>)

Under suitable initialization, the sequence  $\theta_n^{t+1} = F_n(\theta_n^t)$  satisfies

 $\|\theta_n^t - \theta^\star\| \precsim \varepsilon(n, \delta)$  when  $t \succeq \log(1/\varepsilon(n, \delta))$ .

Furthermore, this bound is tight.

Nhat Ho (Univ of Texas, Austin)

<sup>&</sup>lt;sup>2</sup>Sivaraman Balakrishnan, Martin J. Wainwright, Bin Yu. *Statistical guarantees for the EM algorithm: From population to sample-based analysis*. Annals of Statistics, 2017.

## Example of stable and fast operators

•  $\{(X_i, Y_i)\}_{i=1}^n$  are generated from a noisy non-linear regression model of the form

$$Y_i = (X_i \theta^*)^2 + \xi_i, \qquad \text{for } i = 1, \dots, n.$$

where  $|\theta^{\star}| >>> 1$ 

- $\xi_i \sim \mathcal{N}(0,1)$  and  $X_i \sim \mathcal{N}(0,1)$
- We use gradient descent method (GD) to the least-squares loss

うかん 正正 ヘビト・モー・ ふんし

## Example of stable and fast operators

- Population GD operator  $F^{GD}$  is  $FAST(\frac{1}{2})$ -convergent
- Sample GD operator  $F_n^{GD}$  is STA(1)-stable with noise  $\varepsilon(n, \delta) = \sqrt{\frac{\log^4(n/\delta)}{n}}$
- $\bullet~$  Under suitable initialization, the sequence  $\theta_n^{t+1}={\rm F}_n^{\rm GD}(\theta_n^t)$  satisfies

$$|\theta_n^t - \theta^\star| \precsim n^{-1/2}$$
 when  $t \succsim \log(n)$ 

A = A = A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A
A

## General theory: Stable and slow operators

- The population operator F is 1-Lipschitz and is SLOW(β)-convergent
- The empirical operator  $F_n$  is STA( $\gamma$ )-stable for some  $\gamma \in [0, (1 + \beta)^{-1})$

Theorem 2 (Ho et al.,  $2024a^3$ )

Under suitable initialization, the sequence  $\theta_n^{t+1} = F_n(\theta_n^t)$  satisfies

$$\|\theta_n^t - \theta^\star\| \precsim [\varepsilon(n,\delta)]^{\frac{\beta}{1+\beta-\gamma\beta}} \qquad \text{when } t \succsim \varepsilon(n,\delta)^{-\frac{1}{1+\beta-\gamma\beta}}$$

Furthermore, this bound is tight.

The proof for this result relies on an epoch-based localization argument

Nhat Ho (Univ of Texas, Austin)

June 2024 19 / 41

•  $\{(X_i, Y_i)\}_{i=1}^n$  are generated from a noisy non-linear regression model of the form

$$Y_i = (X_i \theta^*)^2 + \xi_i, \qquad \text{for } i = 1, \dots, n$$

where  $\theta^{\star}=0$ 

- $\xi_i \sim \mathcal{N}(0,1)$  and  $X_i \sim \mathcal{N}(0,1)$
- We apply gradient descent method (GD) to the least-squares loss

うかん 正正 ヘビト・モー・ ふんし

• Population GD operator:

$$\mathbf{F}^{\mathrm{GD}}(\theta) = \theta \left[ 1 - 6\eta \theta^2 \right]$$

 $\implies$  F<sup>GD</sup> is SLOW $(\frac{1}{2})$ -convergent as  $\eta \in (0, \frac{1}{6}]$ 

• Sample GD operator:

$$\mathbf{F}_{n}^{\mathrm{GD}}(\theta) = \theta - \eta \left(\frac{2}{n} \sum_{i=1}^{n} X_{i}^{4} \theta^{3} - \frac{2}{n} \sum_{i=1}^{n} Y_{i} X_{i}^{2} \theta\right)$$

 $\Longrightarrow {\rm F}_n^{\rm GD}$  is  ${\rm STA}(1)\text{-stable}$  with noise  $\varepsilon(n,\delta)=\sqrt{\frac{\log^4(n/\delta)}{n}}$ 

 $\bullet~$  Under suitable initialization, the sequence  $\theta_n^{t+1}={\rm F}_n^{\rm GD}(\theta_n^t)$  satisfies

$$|\theta_n^t - \theta^\star| \precsim n^{-1/4}$$
 when  $t \succsim \sqrt{n}$ 

▲□ ▲ □ ▲ ■ ▲ ■ ■ ■ ● ● ●

## General theory: Unstable and fast operators

- The population operator F is FAST( $\kappa$ )-convergent
- The empirical operator  $F_n$  is  $\text{UNS}(\gamma)$ -unstable over the annulus  $\mathbb{A}(\theta^{\star}, \widetilde{\rho}_n, \rho)$  for some  $\gamma < 0$

#### Theorem 3 (Ho et al., 2024a)

Under suitable initialization, the sequence  $\theta_n^{t+1} = F_n(\theta_n^t)$  satisfies

$$\min_{k \in \{0,1,\dots,t\}} \|\theta_n^k - \theta^\star\| \precsim \max\left\{ [\varepsilon(n,\delta)]^{\frac{1}{1+|\gamma|}}, \ \widetilde{\rho}_n \right\} \qquad \textit{when } t \succsim \log(1/\varepsilon(n,\delta)).$$

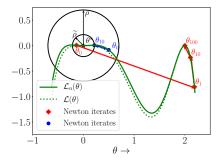
Furthermore, this bound is tight.

000 EIE 4E + 4E + 4

## Necessity of the minimum

• We consider the following example:

$$\mathcal{L}(\theta) = -\theta^4 (\theta - 2)^2$$
 and  $\mathcal{L}_n(\theta) = -\left(\theta^4 - \frac{\theta^2}{\sqrt{n}}\right)(\theta - 2)^2$ 



- When the initialization is too close to  $\theta^*$  (red diamonds), Newton's iterates jump far away from  $\theta^*$  and converge to another fixed point
- When the initialization is in A(θ<sup>\*</sup>, ρ̃, ρ), the Newton iterates (blue circles) do not leave this annulus and converge to a small neighborhood of θ<sup>\*</sup><sub>=</sub>, <sub>= = → Q</sub>

•  $\{(X_i, Y_i)\}_{i=1}^n$  are generated from a noisy non-linear regression model of the form

$$Y_i = (X_i \theta^*)^2 + \xi_i, \qquad \text{for } i = 1, \dots, n$$

where  $\theta^{\star} = 0$ 

- $\xi_i \sim \mathcal{N}(0,1)$  and  $X_i \sim \mathcal{N}(0,1)$
- We apply Newton's method (NM) to the least-squares loss

000 EIE 4E + 4E + 4

• Population NM operator:

$$\mathbf{F}^{\mathrm{NM}}(\theta) = \theta - \frac{\theta^3}{3\theta^2} = \frac{2}{3}\theta$$

 $\implies F^{NM} \text{ is } FAST(\frac{2}{3})\text{-convergent}$ 

• Sample NM operator:

$$\mathbf{F}_{n}^{\mathrm{NM}}(\theta) = \theta - \frac{\left(\frac{1}{n}\sum_{i=1}^{n}X_{i}^{4}\right)\theta^{3} - \left(\frac{1}{n}\sum_{i=1}^{n}Y_{i}X_{i}^{2}\right)\theta}{\left(\frac{3}{n}\sum_{i=1}^{n}X_{i}^{4}\right)\theta^{2} - \frac{1}{n}\sum_{i=1}^{n}Y_{i}X_{i}^{2}}$$

 $\Longrightarrow \mathrm{F}_n^{\mathrm{NM}} \text{ is } \underbrace{\mathrm{UNS}(-1)}_{\rho_n \asymp} \text{ log}(n/\delta)/n^{1/4}$  with  $\widetilde{\rho}_n \asymp \log(n/\delta)/n^{1/4}$ 

000 EIE 4E + 4E + 4

- $F^{NM}$  is  $FAST(\frac{2}{3})$ -convergent
- $F_n^{\rm NM}$  is UNS(-1)-unstable over the annulus  $\mathbb{A}(\theta^\star, \tilde{\rho}_n, 1)$  with  $\tilde{\rho}_n \asymp \log(n/\delta)/n^{1/4}$
- Under suitable initialization, the sequence  $\theta_n^{t+1} = F_n^{NM}(\theta_n^t)$  satisfies

$$|\theta_n^t - \theta^\star| \precsim n^{-1/4}$$
 when  $t \succeq \log(n)$ 

> < = > < = > = = = < < <

## General theory: Unstable and slow operators

- The population operator F is 1-Lipschitz and is SLOW(β)-convergent
- The empirical operator  $F_n$  is  $\text{UNS}(\gamma)$ -unstable over the annulus  $\mathbb{A}(\theta^{\star}, \widetilde{\rho}_n, \rho)$  for some  $\gamma < 0$

#### Theorem 4 (Ho et al., 2024a)

Under suitable initialization, the sequence  $\theta_n^{t+1} = F_n(\theta_n^t)$  satisfies

$$\min_{k \in \{0,1,\dots,t\}} \|\theta_n^k - \theta^\star\| \precsim \max\left\{ [\varepsilon(n,\delta)]^{\frac{\beta}{1+\beta-\gamma\beta}}, \ \widetilde{\rho}_n \right\} \qquad \text{when } t \succsim \varepsilon(n,\delta)^{-\frac{1}{1+\beta}}.$$

Furthermore, this bound is tight.

▲□ ▲ □ ▲ ■ ▲ ■ ■ ■ ● ● ●

•  $\{(X_i, Y_i)\}_{i=1}^n$  are generated from a noisy non-linear regression model of the form

$$Y_i = (X_i \theta^*)^2 + \xi_i, \qquad \text{for } i = 1, \dots, n$$

where  $\theta^{\star} = 0$ 

- $\xi_i \sim \mathcal{N}(0,1)$  and  $X_i \sim \mathcal{N}(0,1)$
- We apply cubic-regularized Newton's method (CNM) to the least-squares loss

▲□ ▲ □ ▲ ■ ▲ ■ ■ ■ ● ● ●

- $\widetilde{\mathcal{L}}$  and  $\widetilde{\mathcal{L}}_n$  are population and sample least-square losses
- Population CNM operator:

$$F^{\text{CNM}}(\theta) = \operatorname*{arg\,min}_{y \in \mathbb{R}} \left\{ \widetilde{\mathcal{L}}'(\theta)(y-\theta) + \frac{1}{2}\widetilde{\mathcal{L}}''(\theta)(y-\theta)^2 + L |y-\theta|^3 \right\}$$
$$= \theta - \frac{\frac{2}{3}\theta^3}{\theta^2 + \sqrt{\theta^4 + \frac{2}{3}\theta^3}}$$

 $\implies F^{\rm CNM}$  is SLOW(2)-convergent

Sample CNM operator:

$$\mathbf{F}_{n}^{\mathrm{CNM}}(\theta) = \operatorname*{arg\,min}_{y \in \mathbb{R}} \left\{ \widetilde{\mathcal{L}}_{n}'(\theta)(y-\theta) + \frac{1}{2} \widetilde{\mathcal{L}}_{n}''(\theta)(y-\theta)^{2} + L \left| y - \theta \right|^{3} \right\}$$

 $\Longrightarrow \mathrm{F}_n^{\mathrm{CNM}} \text{ is } \frac{\mathrm{UNS}(-\frac{1}{2})}{\mathrm{enstable}} \text{ over the annulus } \mathbb{A}(\theta^\star, \widetilde{\rho}_n, 1) \text{ with } \widetilde{\rho}_n \asymp \ \log(n/\delta)/n^{1/4}$ 

- F<sup>CNM</sup> is SLOW(2)-convergent
- $\mathbf{F}_n^{\mathrm{CNM}}$  is  $\mathrm{UNS}(-\frac{1}{2})$ -unstable over the annulus  $\mathbb{A}(\theta^\star, \widetilde{\rho}_n, 1)$  with  $\widetilde{\rho}_n \asymp \log(n/\delta)/n^{1/4}$
- Under suitable initialization, the sequence  $\theta_n^{t+1} = F_n^{\text{CNM}}(\theta_n^t)$  satisfies

$$|\theta_n^t - \theta^\star| \precsim n^{-1/4}$$
 when  $t \succsim n^{1/6}$ 

000 EIE 4E + 4E + 4

# Summary of results

<b>Operator Properties</b>	Optimization Rate	Stability	Iterations for convergence	Statistical error on convergence
General expressions				
Fast, stable	$FAST(\kappa)$	$STA(\gamma)$	$\log(1/\varepsilon(n,\delta))$	$\varepsilon(n,\delta)$
Slow, stable	$SLOW(\beta)$	$STA(\gamma)$	$\varepsilon(n,\delta)^{-\frac{1}{1+\beta-\gamma\beta}}$	$[\varepsilon(n,\delta)]^{rac{eta}{1+eta-\gammaeta}}$
Fast, unstable	$FAST(\kappa)$	$\text{UNS}(\gamma)$	$\log(1/\varepsilon(n,\delta))$	$[\varepsilon(n,\delta)]^{\frac{1}{1+ \gamma }}$
Slow, unstable	$SLOW(\beta)$	$\text{UNS}(\gamma)$	$[\varepsilon(n,\delta)]^{-\frac{1}{1+\beta}}$	$[\varepsilon(n,\delta)]^{\frac{\beta}{1+\beta+ \gamma \beta}}$

Nhat Ho (Univ of Texas, Austin)

Exponentially increasing step size gradient descent (EGD)

- Using gradient descent (GD) with fixed or decaying step-size is a standard practice
- Such step-size schedules can be sub-optimal in computational complexity for reaching final statistical radius when the loss functions are locally convex
- In (Ho et al., 2024b<sup>4</sup>), we demonstrate that exponentially increasing the step size can indeed give optimal computational complexity O(nd) for parameter estimation

<sup>4</sup>Nhat Ho, Tongzheng Ren, Purnamrita Sarkar, Sujay Sanghavi, Rachel Ward ( $\alpha$ - $\beta$  order). An exponentially increasing step-size for parameter estimation in statistical models. Under revision, Journal of Machine Learning Research, 2024 ( $\equiv \Rightarrow e \equiv \Rightarrow \equiv \Rightarrow \circ \circ \circ$ )

Nhat Ho (Univ of Texas, Austin)

Exponentially increasing step size gradient descent (EGD)

• The sample EGD updates take the form:

$$\theta_n^{t+1} := \theta_n^t - \frac{\eta}{\tau^t} \nabla f_n(\theta_n^t),$$

where  $f_n$  is the sample loss function,  $\tau \in (0,1]$  is some given scale parameter, and  $\eta > 0$  is the step size

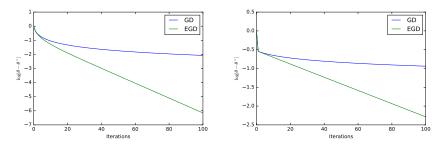
• The corresponding population EGD updates are:

$$\theta^{t+1} := \theta^t - \frac{\eta}{\tau^t} \nabla f(\theta^t)$$

where f is the population loss function

4 3 4 3 4 3 4

## Fixed scale $\tau$ : Insights from simple convex settings



GD versus EGD iterates for solving the population loss function  $f(\theta) = \theta^{2p}/(2p)$ when  $p \in \{2, 4\}$ . Left: p = 2; Right: p = 4. The EGD iterates converge linearly to the true parameter  $\theta^* = 0$ , while the GD iterates converge to  $\theta^*$  at a sub-linear rate.

## Fixed scale $\tau$ : Linear convergence of population EGD

• Homogeneity Assumption: There exist constants  $\alpha \ge 0$  and  $\rho > 0$  such that f is locally convex in  $\mathcal{B}(\theta^*, \rho)$  and for all  $\theta \in \mathbb{B}(\theta^*, \rho)$ , we have

$$\begin{aligned} \lambda_{\max}(\nabla^2 f(\theta)) &\leq c_1 \|\theta - \theta^*\|^{\alpha}, \\ \|\nabla f(\theta)\| &\geq c_2 (f(\theta) - f(\theta^*))^{1 - \frac{1}{\alpha + 2}}, \end{aligned}$$

where  $c_1, c_2$  are some positive universal constants

#### Theorem 5 (Ho et al., 2024b)

Assume that the homogeneity assumption holds for some  $\alpha > 0$ . For  $\tau \in [0, 1)$ such that  $\frac{1-\tau^{\frac{\alpha+2}{\alpha}}}{\tau} \leq \frac{c_2^{\alpha+1}}{2c_1(\alpha+2)^{\alpha}}$ , the population EGD iterates  $\{\theta^t\}_{t\geq 0}$  satisfy  $f(\theta^t) - f(\theta^*) \precsim \tau^{\frac{\alpha+2}{\alpha}t},$  $\|\theta^t - \theta^*\| \precsim \tau^{\frac{t}{\alpha}}.$ 

< ロ > < 同 > < 三 > < 三 > < 三 > < 三 > < 回 > < ○ < ○ </p>

Optimal complexities of sample EGD when  $\alpha \geq 1$ 

• Stability of gradient condition: For  $\bar{\gamma} \ge 0$ ,

$$\sup_{\theta \in \mathbb{B}(\theta^*, r)} \left\| \nabla f_n(\theta) - \nabla f(\theta) \right\| \precsim r^{\bar{\gamma}} \varepsilon(n, \delta),$$

for any r > 0

#### Theorem 6 (Ho et al., 2024b)

Assume the homogeneity and stability conditions hold with  $\alpha \geq \bar{\gamma} \geq 1$ . Under suitable assumptions, we have

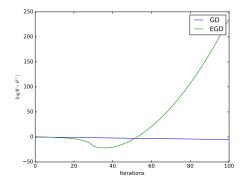
$$\min_{1 \le k \le t} \|\theta_n^k - \theta^*\| \precsim (\varepsilon(n,\delta))^{\frac{1}{\alpha+1-\bar{\gamma}}} \qquad \textit{when} \qquad t \succsim \log(1/\varepsilon(n,\delta)).$$

- The fixed-step size GD iterates reach the similar statistical radius after  $\mathcal{O}(\varepsilon(n, \delta)^{-\frac{\alpha}{\alpha+1-\overline{\gamma}}})$  number of iterations
- The total computational complexity of the EGD is optimal and much cheaper than that of the GD

▲□▶ ▲□▶ ▲ヨ▶ ▲ヨ▶ ヨヨ ののべ

## Fixed scale $\tau$ : Divergence under local strong convexity

- Our results thus far are under the homogeneity assumption when  $\alpha > 0$
- When  $\alpha = 0$ , i.e., the population loss is locally strongly convex, the population EGD iterates diverge



GD and EGD algorithm iterates for solving  $f(\theta) = \theta^2/2$ . EGD iterates converge faster than GD at the first several iterations, and start to diverge.

(4) (3) (4) (4) (4)

## Fixed scale $\tau$ : Statistical guarantee when $\alpha = 0$

#### Theorem 7 (Ho et al., 2024b)

Assume that the homogeneous and the stability conditions hold with  $\alpha = \bar{\gamma} = 0$ . Then, by choosing  $\bar{T} \simeq \log(1/(\eta))/\log(1/\tau)$ , we have

$$\min_{1 \le t \le \bar{T}} \|\theta_n^t - \theta^*\| \precsim \underbrace{\varepsilon(n, \delta)}_{Statistical \ error} + \underbrace{\exp\left(-\frac{(1 - \eta c_1)(\tau^{-1} - c_1\eta)}{2(\tau^{-2} - 1)}\right) \|\theta_n^0 - \theta^*\|}_{Optimization \ error},$$

where  $c_1$  is constant in the homogeneity assumption.

- Similar to the population EGD iterates, after  $\bar{T} \asymp \log(1/(\eta))/\log(1/\beta)$  iterations, the sample EGD iterates diverge
- $\bullet\,$  The non-vanishing optimization error can be resolved by using sample size dependent scale  $\tau\,$

▲□ ▲ □ ▲ ■ ▲ ■ ■ ■ ● ● ●

## Optimality of EGD with sample size dependent scale $\tau$

- We choose the scale au to balance the statistical and optimization errors
- It leads to  $\tau^2 = 1 \frac{(1-\eta c_1)^2}{2\log(1/\varepsilon(n,\delta))}$  where  $c_1$  is a constant in the homogeneity assumption

#### Theorem 8 (Ho et al., 2024b)

Given that choice of  $\tau$ , we have:

(a) When  $\alpha = 0$  and  $\bar{\gamma} = 0$  in homogeneity and stability conditions:

 $\min_{1 \leq k \leq t} \|\theta_n^t - \theta^*\| \precsim \varepsilon(n,\delta) \qquad \textit{when} \quad t \succsim \log(1/\varepsilon(n,\delta))$ 

(b) When  $\alpha \geq \bar{\gamma} \geq 1$  in homogeneity and stability conditions:

 $\min_{1 \leq k \leq t} \|\theta_n^k - \theta^*\| \precsim (\varepsilon(n,\delta))^{\frac{1}{\alpha+1-\bar{\gamma}}} \qquad \textit{when} \qquad t \succsim \log(1/\varepsilon(n,\delta)).$ 

Therefore, with the sample size dependent scale τ, the EGD has optimal computational complexity O(nd) to reach the final statistical radii

## Future directions

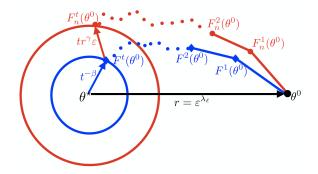
- Accelerated optimization methods, such as Nesterov gradient descent, cannot be analyzed directly by the current framework
  - It is due to the multi-variables operators associated with accelerated optimization methods
- The theory does not extend to the setting of dependent data (the population operator is not naturally defined)
- There are three practical directions for the exponentially increasing step size gradient descent method:
  - Beyond the homogeneity condition
  - Tuning free of step size (e.g., RMSProp)
  - Global convergence (e.g., Moreau-Yosida regularization via Hamilton-Jacobi PDE)

▲□ ▲ □ ▲ ■ ▲ ■ ■ ■ ● ● ●

#### Thank You!

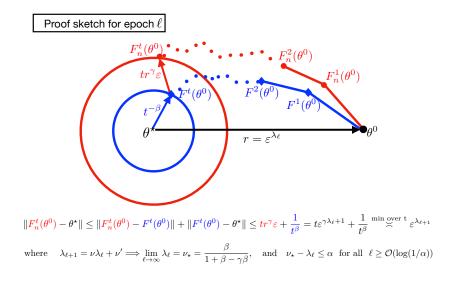
## Outline of proof: Epoch-based argument

- Assume  $\theta^0$  the starting point for epoch  $\ell$  and  $r = \|\theta^{\star} \theta^0\| = \varepsilon(n, \delta)^{\lambda_{\ell}}$
- $\bullet$  Slow convergence of population iterates:  $\|F^t(\theta^0)-\theta^\star\|\precsim t^{-\beta}$
- Stability of sample operator:  $\|F_n^t(\theta^0) F^t(\theta^0)\| \precsim t \cdot r^{\gamma} \cdot \varepsilon$



• **Goal:** At the end of epoch  $\ell$ , we want to find suitable t and  $\lambda_{\ell+1}$  such that  $\|F_n^t(\theta^0) - \theta^\star\| \precsim \varepsilon^{\lambda_{\ell+1}}$ 

## Outline of proof: Epoch-based argument



## Outline of proof

- Assume that  $\|\theta_n^t \theta^\star\| > [\varepsilon(n, \delta)]^{\frac{1}{1+|\gamma|}}$  for all  $t \precsim \log(1/\varepsilon(n, \delta))$
- As F is FAST( $\kappa$ )-convergent and  $F_n$  is UNS( $\gamma$ )-unstable,

$$\begin{aligned} \theta_n^{t+1} - \theta^{\star} \| &\leq \|F_n(\theta_n^t) - F(\theta_n^t)\| + \|F(\theta_n^t) - \theta^{\star}\| \\ &\leq \varepsilon(n, \delta) \max\left\{\frac{1}{[\varepsilon(n, \delta)]^{\frac{|\gamma|}{1+|\gamma|}}}, \rho\right\} + \kappa \cdot \|\theta_n^t - \theta^{\star}\| \end{aligned}$$

$$\leq \varepsilon(n,\delta) \max\left\{\frac{1}{[\varepsilon(n,\delta)]^{\frac{|\gamma|}{1+|\gamma|}}},\rho\right\} (1+\kappa+\ldots+\kappa^{t-1}) \\ +\kappa^t \cdot \|\theta_n^0 - \theta^\star\| \\ \precsim [\varepsilon(n,\delta)]^{\frac{1}{1+|\gamma|}},$$

when  $t \succsim \log(1/\varepsilon(n,\delta))$ 

. . .

## Outline of proof

• 
$$\nu_{\star} = \frac{\beta}{1+\beta-\gamma\beta}$$

• Assume that  $\|\theta_n^t - \theta^\star\| > \max\left\{ [\varepsilon(n, \delta)]^{\nu_\star}, \ \widetilde{\rho}_n \right\}$  for all  $t \preceq \varepsilon(n, \delta)^{-\frac{1}{1+\beta}}$ 

• As F is SLOW( $\beta$ )-convergent and  $F_n$  is UNS( $\gamma$ )-unstable,

$$\begin{aligned} \|\theta_n^{t+1} - \theta^\star\| &\leq \frac{1}{t^\beta} + t \cdot \frac{\varepsilon(n,\delta)}{[\varepsilon(n,\delta)]^{\nu_\star |\gamma|}} \\ &\precsim [\varepsilon(n,\delta)]^{\nu_\star}, \end{aligned}$$

when  $t \succeq \varepsilon(n, \delta)^{-\frac{1}{1+\beta}}$ 

< □ > < 同 >

## Additional regularity condition to remove the minimum

- The population operator F is FAST( $\kappa$ )-convergent
- The empirical operator  $F_n$  is  $\text{UNS}(\gamma)$ -unstable over the annulus  $\mathbb{A}(\theta^{\star}, \widetilde{\rho}_n, \rho)$  for some  $\gamma < 0$
- There exists a constant C such that the sequence  $\theta_n^t = F_n^t(\theta_n^0)$  satisfies:

$$\|\theta_n^{t+1} - \theta^\star\| \le C\widetilde{\rho} \quad \text{whenever} \quad \|\theta_n^t - \theta^\star\| \le \widetilde{\rho},$$

where 
$$\widetilde{\rho} = \max\left\{ [\varepsilon(n,\delta)]^{\frac{1}{1+|\gamma|}}, \ \widetilde{\rho}_n \right\}$$

#### **Proposition 9**

Under suitable initialization, the sequence  $\theta_n^{t+1} = F_n(\theta_n^t)$  satisfies

$$\|\theta_n^t - \theta^\star\| \precsim \max\left\{[\varepsilon(n,\delta)]^{\frac{1}{1+|\gamma|}}, \ \widetilde{\rho}_n\right\} \qquad \textit{when } t \succsim \log(1/\varepsilon(n,\delta)).$$

Furthermore, this bound is tight.

▲□▶ ▲□▶ ▲□▶ ▲□▶ 三回 ののの