The Power of Adaptivity in SGD: Self-Tuning Step Sizes with Unbounded Gradients and Affine Variance

Speaker: Matthew Faw

Authors: F*, Isidoros Tziotis*, Constantine Caramanis, Aryan Mokhtari, Sanjay Shakkottai, Rachel Ward The University of Texas at Austin





Find a first-order stationary point of a non-convex, *L*-smooth function *F*.

Stochastic Gradient Descent

 $w_{t+1} = w_t - \eta_t g_t$

Find a first-order stationary point of a non-convex, *L*-smooth function *F*.

Stochastic Gradient Descent

 $w_{t+1} = w_t - \eta_t g_t$

- $\mathbb{E}[g] = \nabla F(w)$ (unbiased stochastic gradient)
- $\mathbb{E}[\|g \nabla F(w)\|^2] \le \sigma_0^2$ (bounded variance)

Find a first-order stationary point of a non-convex, *L*-smooth function *F*.

Stochastic Gradient Descent

$$w_{t+1} = w_t - \eta_t g_t \qquad \eta_t = \min\left\{\frac{1}{L}, \frac{c}{\sqrt{T}\sigma_0}\right\}$$

- $\mathbb{E}[g] = \nabla F(w)$ (unbiased stochastic gradient)
- $\mathbb{E}[\|g \nabla F(w)\|^2] \le \sigma_0^2$ (bounded variance)

Find a first-order stationary point of a non-convex, *L*-smooth function *F*.

Stochastic Gradient Descent

$$w_{t+1} = w_t - \eta_t g_t \qquad \eta_t = \min\left\{\frac{1}{L(1+\sigma_1^2)}, \frac{c}{\sqrt{T}\sigma_0}\right\}$$

- $\mathbb{E}[g] = \nabla F(w)$ (unbiased stochastic gradient)
- $\mathbb{E}[\|g \nabla F(w)\|^2] \le \sigma_0^2 + \sigma_1^2 \|\nabla F(w)\|^2$ (affine variance)

Find a first-order stationary point of a non-convex, *L*-smooth function *F*.

Stochastic Gradient Descent

$$w_{t+1} = w_t - \eta_t g_t \qquad \eta_t = \min\left\{\frac{1}{L(1+\sigma_1^2)}, \frac{c}{\sqrt{T}\sigma_0}\right\}$$

Achieves $\min_{t} \|\nabla F(w_t)\|^2 = O(1/\sqrt{T})$ convergence rate under the following assumptions:

- $\mathbb{E}[g] = \nabla F(w)$ (unbiased stochastic gradient)
- $\mathbb{E}[\|g \nabla F(w)\|^2] \le \sigma_0^2 + \sigma_1^2 \|\nabla F(w)\|^2$ (affine variance)

Can **oscillate** or **diverge** if *L* or σ_1^2 is underestimated!

Find a first-order stationary point of a non-convex, *L*-smooth function *F*.

Stochastic Gradient Descent

$$w_{t+1} = w_t - \eta_t g_t \qquad \eta_t = \min\left\{\frac{1}{L(1+\sigma_1^2)}, \frac{c}{\sqrt{T}\sigma_0}\right\}$$

Achieves $\min_{t} \|\nabla F(w_t)\|^2 = O(1/\sqrt{T})$ convergence rate under the following assumptions:

- $\mathbb{E}[g] = \nabla F(w)$ (unbiased stochastic gradient)
- $\mathbb{E}[\|g \nabla F(w)\|^2] \le \sigma_0^2 + \sigma_1^2 \|\nabla F(w)\|^2$ (affine variance)

Can **oscillate** or **diverge** if *L* or σ_1^2 is underestimated!

Does **not** recover improved O(1/T) rate when σ_0^2 is small and unknown!

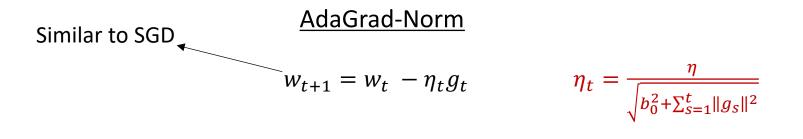
Find a first-order stationary point of a non-convex, *L*-smooth function *F*.

AdaGrad-Norm

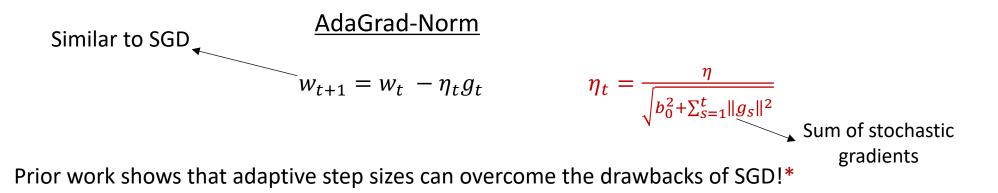
$$w_{t+1} = w_t - \eta_t g_t$$
 $\eta_t = \frac{\eta}{\sqrt{b_0^2 + \sum_{s=1}^t ||g_s||^2}}$

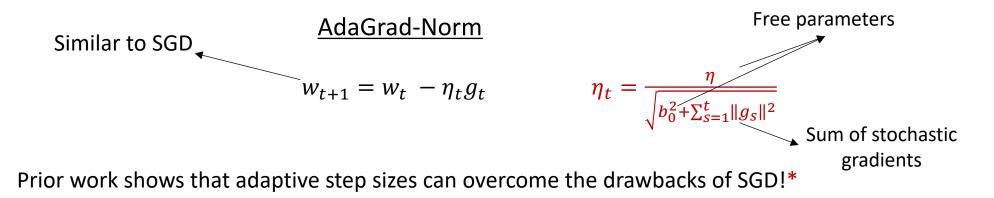
Prior work shows that adaptive step sizes can overcome the drawbacks of SGD!*

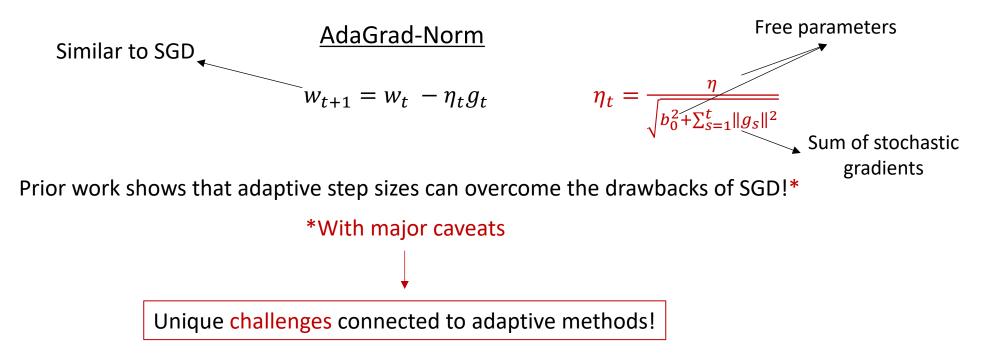
Find a first-order stationary point of a non-convex, *L*-smooth function *F*.



Prior work shows that adaptive step sizes can overcome the drawbacks of SGD!*







- **i. Challenge 1**: Bias + Affine Variance
 - Step size η_t depends on past and current stochastic gradients.

- i. Challenge 1: Bias + Affine Variance
 - Step size η_t depends on past and current stochastic gradients.

- i. Challenge 1: Bias + Affine Variance
 - Step size η_t depends on past and current stochastic gradients.
 - Especially challenging in presence of affine variance.

 $\mathbb{E}_{t}[\eta_{t}] \|\nabla F(w_{t})\|^{2} \leq \mathbb{E}_{t}[F(w_{t}) - F(w_{t+1})] + c \cdot \mathbb{E}_{t}[\eta_{t}^{2} \|g_{t}\|^{2}]$

- i. Challenge 1: Bias + Affine Variance
 - Step size η_t depends on past and current stochastic gradients.

Large $\sigma_1 \Rightarrow$ techniques from bounded variance regimes

completely break!

• Especially challenging in presence of affine variance.

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}_t[\eta_t] \|\nabla F(w_t)\|^2 \le \mathbb{E}_t[F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t[\eta_t^2 \|g_t\|^2]$

- i. Challenge 1: Bias + Affine Variance
 - Step size η_t depends on past and current stochastic gradients.

Large $\sigma_1 \implies$ techniques from bounded variance regimes completely break!

Especially challenging in presence of affine variance.

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}_t[\eta_t] \|\nabla F(w_t)\|^2 \le \mathbb{E}_t[F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t[\eta_t^2 \|g_t\|^2]$

- ii. Challenge 2: Step size scaling
 - Can no longer guarantee deterministically that $\eta_t \sim 1/\sqrt{T}$.
 - Depends inversely on $\sum_t ||g_t||^2$.

- i. Challenge 1: Bias + Affine Variance
 - Step size η_t depends on past and current stochastic gradients.

Large $\sigma_1 \Rightarrow$ techniques from bounded variance regimes completely break!

Especially challenging in presence of affine variance.

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}_t[\eta_t] \|\nabla F(w_t)\|^2 \le \mathbb{E}_t[F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t[\eta_t^2 \|g_t\|^2]$

- ii. Challenge 2: Step size scaling
 - Can no longer guarantee deterministically that $\eta_t \sim 1/\sqrt{T}$.
 - Depends inversely on $\sum_t ||g_t||^2$.



1. "Bias-free" – [Li-Orabona'19,'20; Savarese-McAllester-Babu-Maire'21; ...]

- 1. "Bias-free" [Li-Orabona'19,'20; Savarese-McAllester-Babu-Maire'21; ...]
 - $\eta_t = \frac{\eta}{\sqrt{b_0^2 + \sum_{s=1}^{t-1} ||g_s||^2}} \Longrightarrow \eta_t$ conditionally independent of $g_t!$
 - Automatically achieves faster convergence when σ_0 is small (unlike SGD).
 - Needs knowledge of *L* for convergence guarantee (like SGD).

Stochastic Optimization with Adaptive Step Sizes – Prior Work

- 1. "Bias-free" [Li-Orabona'19,'20; Savarese-McAllester-Babu-Maire'21; ...]
 - $\eta_t = \frac{\eta}{\sqrt{b_0^2 + \sum_{s=1}^{t-1} ||g_s||^2}} \Longrightarrow \eta_t$ conditionally independent of g_t !
 - Automatically achieves faster convergence when σ_0 is small (unlike SGD).
 - **Needs knowledge of** *L* for convergence guarantee (like SGD).
- 2. "Bounded gradients" [Ward-Wu-Bottou'19; Kavis-Levy-Bach-Cevher'19; Défossez-Bottou-Bach-Usunier'20; ...]

Stochastic Optimization with Adaptive Step Sizes – Prior Work

- 1. "Bias-free" [Li-Orabona'19,'20; Savarese-McAllester-Babu-Maire'21; ...]
 - $\eta_t = \frac{\eta}{\sqrt{b_0^2 + \sum_{s=1}^{t-1} ||g_s||^2}} \Longrightarrow \eta_t$ conditionally independent of g_t !
 - Automatically achieves faster convergence when σ_0 is small (unlike SGD).
 - Needs knowledge of *L* for convergence guarantee (like SGD).
- 2. "Bounded gradients" [Ward-Wu-Bottou'19; Kavis-Levy-Bach-Cevher'19; Défossez-Bottou-Bach-Usunier'20; ...]
 - Develop techniques to bound bias.
 - Converges w/o knowing *L* or σ_0 .
 - But relies on **uniform gradient bounds** $\sup_{w \in \mathbb{R}^d} \|\nabla F(w)\|^2 \le B < \infty$

- 1. "Bias-free" [Li-Orabona'19,'20; Savarese-McAllester-Babu-Maire'21; ...]
 - $\eta_t = \frac{\eta}{\sqrt{b_0^2 + \sum_{s=1}^{t-1} ||g_s||^2}} \Longrightarrow \eta_t$ conditionally independent of g_t !
 - Automatically achieves faster convergence when σ_0 is small (unlike SGD).
 - Needs knowledge of *L* for convergence guarantee (like SGD).
- 2. "Bounded gradients" [Ward-Wu-Bottou'19; Kavis-Levy-Bach-Cevher'19; Défossez-Bottou-Bach-Usunier'20; ...]
 - Develop techniques to bound bias.
 - Converges w/o knowing *L* or σ_0 .
 - But relies on **uniform gradient bounds** $\sup_{w \in \mathbb{R}^d} \|\nabla F(w)\|^2 \le B < \infty$

- 1. "Bias-free" [Li-Orabona'19,'20; Savarese-McAllester-Babu-Maire'21; ...]
 - $\eta_t = \frac{\eta}{\sqrt{b_0^2 + \sum_{s=1}^{t-1} ||g_s||^2}} \Longrightarrow \eta_t$ conditionally independent of g_t !
 - Automatically achieves faster convergence when σ_0 is small (unlike SGD).
 - Needs knowledge of *L* for convergence guarantee (like SGD).
- 2. "Bounded gradients" [Ward-Wu-Bottou'19; Kavis-Levy-Bach-Cevher'19; Défossez-Bottou-Bach-Usunier'20; ...]
 - Develop techniques to bound bias.
 - Converges w/o knowing *L* or σ_0 .

3.

- But relies on **uniform gradient bounds** $\sup_{w \in \mathbb{R}^d} \|\nabla F(w)\|^2 \le B < \infty$
- "Bounded variance with light noise" [Kavis-Levy-Cevher'22]

- 1. "Bias-free" [Li-Orabona'19,'20; Savarese-McAllester-Babu-Maire'21; ...]
 - $\eta_t = \frac{\eta}{\sqrt{b_0^2 + \sum_{s=1}^{t-1} ||g_s||^2}} \Longrightarrow \eta_t$ conditionally independent of $g_t!$
 - Automatically achieves faster convergence when σ_0 is small (unlike SGD).
 - Needs knowledge of *L* for convergence guarantee (like SGD).
- 2. "Bounded gradients" [Ward-Wu-Bottou'19; Kavis-Levy-Bach-Cevher'19; Défossez-Bottou-Bach-Usunier'20; ...]
 - Develop techniques to bound bias.
 - Converges w/o knowing *L* or σ_0 .
 - But relies on **uniform gradient bounds** $\sup_{w \in \mathbb{R}^d} \|\nabla F(w)\|^2 \le B < \infty$

- 3. "Bounded variance with light noise" [Kavis-Levy-Cevher'22]
 - Develop techniques to bound bias.
 - Converges w/o knowing *L* or σ_0 .
 - Requires noise $||g| \nabla F(w)||^2$ to be **uniformly sub-Gaussian** (\Rightarrow bounded variance).

Stochastic Optimization with Adaptive Step Sizes – Prior Work

Three main lines of Prior Work (**uniformly-bounded** variance):

- 1. "Bias-free" [Li-Orabona'19,'20; Savarese-McAllester-Babu-Maire'21; ...]
 - $\eta_t = \frac{\eta}{\sqrt{b_0^2 + \sum_{s=1}^{t-1} ||g_s||^2}} \Longrightarrow \eta_t$ conditionally independent of $g_t!$
 - Automatically achieves faster convergence when σ_0 is small (unlike SGD). ٠
 - **Needs knowledge of** *L* for convergence guarantee (like SGD). •
- 2. "Bounded gradients" [Ward-Wu-Bottou'19; Kavis-Levy-Bach-Cevher'19; Défossez-Bottou-Bach-Usunier'20; ...]
 - Develop techniques to bound bias. •
 - Converges w/o knowing L or σ_0 . ٠
 - But relies on **uniform gradient bounds** sup $\|\nabla F(w)\|^2 \le B < \infty$ • $w \in \mathbb{R}^d$

- "Bounded variance with light noise" [Kavis-Levy-Cevher'22] 3.
 - Develop techniques to bound bias. ٠
 - Converges w/o knowing L or σ_0 . •
 - **No** prior proof techniques extend to the **affine variance** case $\mathbb{E}[||g \nabla F(w)||^2] \leq \sigma_0^2 + \sigma_1^2 ||\nabla F(w)||^2$ Requires noise $||g - \nabla F(w)||^2$ to be **uniformly sub-Gaussian** (\Rightarrow bounded variance). •

Question

Is there an adaptive method which:

- Converges at an $\tilde{O}\left(\frac{1}{\sqrt{T}}\right)$ rate under same assumptions as SGD?
 - $\mathbb{E}[g] = \nabla F(w)$ (unbiased stochastic gradient)
 - $\mathbb{E}[\|g \nabla F(w)\|^2] \le \sigma_0^2 + \sigma_1^2 \|\nabla F(w)\|^2$ (affine variance)
- Requires no knowledge of L, σ_0 , or σ_1 ?

Question

Is there an adaptive method which:

- Converges at an $\tilde{O}\left(\frac{1}{\sqrt{T}}\right)$ rate under same assumptions as SGD?
 - $\mathbb{E}[g] = \nabla F(w)$ (unbiased stochastic gradient)
 - $\mathbb{E}[\|g \nabla F(w)\|^2] \le \sigma_0^2 + \sigma_1^2 \|\nabla F(w)\|^2$ (affine variance)
- Requires no knowledge of L, σ_0 , or σ_1 ?



- **Challenge 1**: Bias + affine variance
 - A key inequality may be *vacuous*:

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}[\eta_t] \|\nabla F(w_t)\|^2 \le \mathbb{E}_t [F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t [\eta_t^2 \|g_t\|^2]$

- **Challenge 1**: Bias + affine variance
 - A key inequality may be *vacuous*:

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}[\eta_t] \|\nabla F(w_t)\|^2 \le \mathbb{E}_t [F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t [\eta_t^2 \|g_t\|^2]$

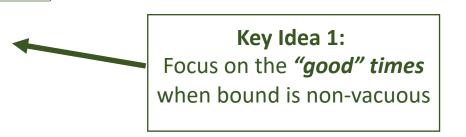
Key Idea 1: Focus on the *"good" times* when bound is non-vacuous

• **Challenge 1**: Bias + affine variance

 \geq

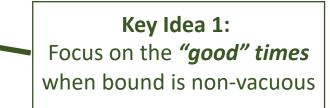
• A key inequality may be *vacuous*:

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}[\eta_t] \| \nabla F(w_t) \|^2 \le \mathbb{E}_t [F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t [\eta_t^2 \| g_t \|^2]$



- **Challenge 1**: Bias + affine variance
 - A key inequality may be *vacuous:*

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}[\eta_t] \|\nabla F(w_t)\|^2 \le \mathbb{E}_t [F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t [\eta_t^2 \|g_t\|^2]$

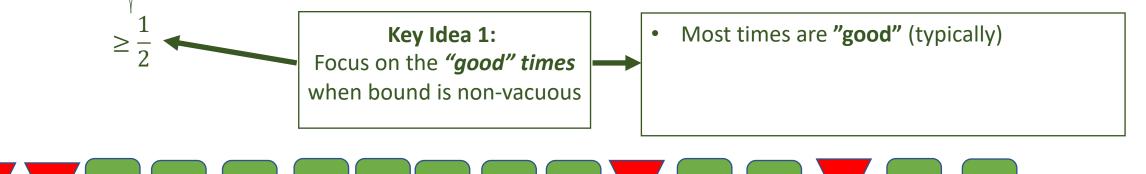






- **Challenge 1**: Bias + affine variance
 - A key inequality may be *vacuous*:

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}[\eta_t] \|\nabla F(w_t)\|^2 \le \mathbb{E}_t [F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t [\eta_t^2 \|g_t\|^2]$

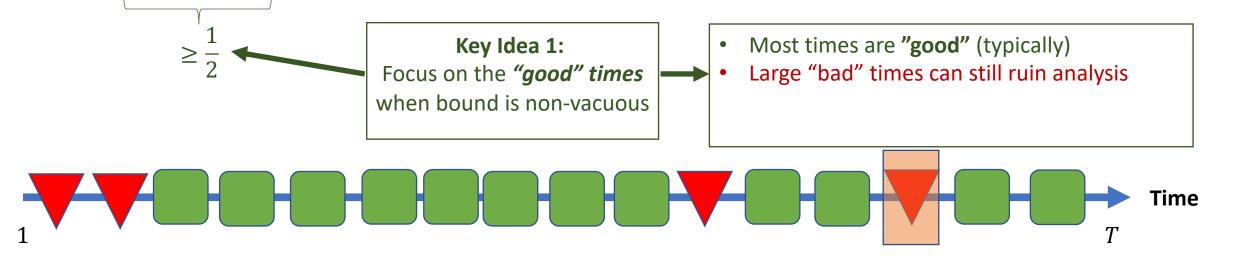






- **Challenge 1**: Bias + affine variance
 - A key inequality may be *vacuous*:

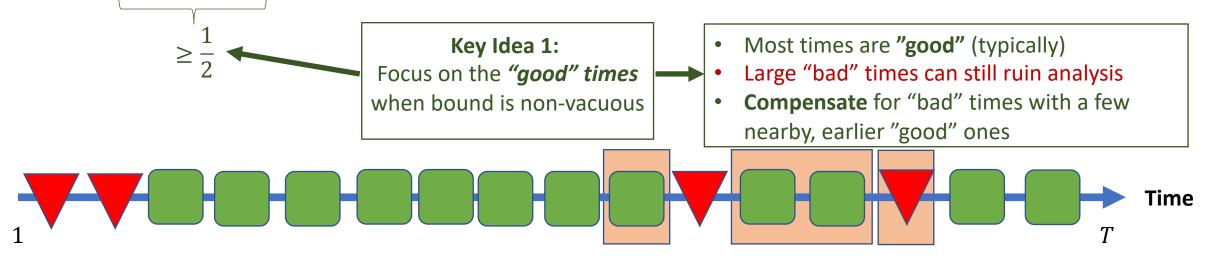
 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}[\eta_t] \|\nabla F(w_t)\|^2 \leq \mathbb{E}_t [F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t [\eta_t^2 \|g_t\|^2]$





- **Challenge 1**: Bias + affine variance
 - A key inequality may be *vacuous*:

 $(1 - \sigma_1 \cdot bias_t) \mathbb{E}[\eta_t] \| \nabla F(w_t) \|^2 \le \mathbb{E}_t [F(w_t) - F(w_{t+1})] + c \cdot \mathbb{E}_t [\eta_t^2 \| g_t \|^2]$





- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$

- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$

Key Idea 2: Recursively improve crude bound on $\mathbb{E}[\sum ||\nabla F(w_t)||^2]$

- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$

Key Idea 2: Recursively improve crude bound on $\mathbb{E}[\sum ||\nabla F(w_t)||^2]$

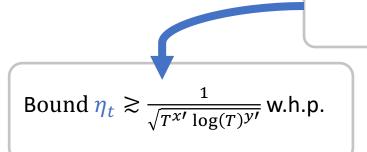
Start with a crude, polynomial bound $\sum_{t} \mathbb{E}[\|\nabla F(w_t)\|^2] \lesssim T^x \log(T)^y$

Obtained via *smoothness* + *unit-step* property of AdaGrad

- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$

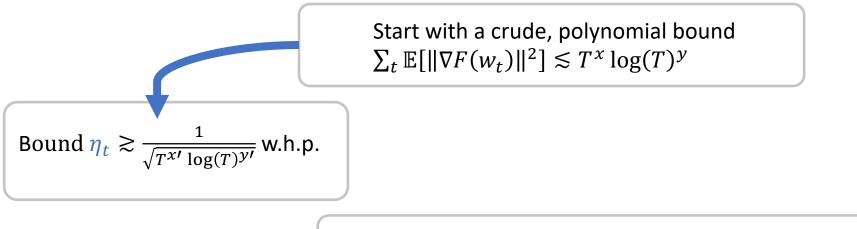
Key Idea 2: Recursively improve crude bound on $\mathbb{E}[\sum \|\nabla F(w_t)\|^2]$

Start with a crude, polynomial bound $\sum_{t} \mathbb{E}[\|\nabla F(w_t)\|^2] \leq T^x \log(T)^y$



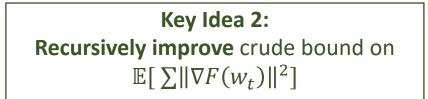
- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$

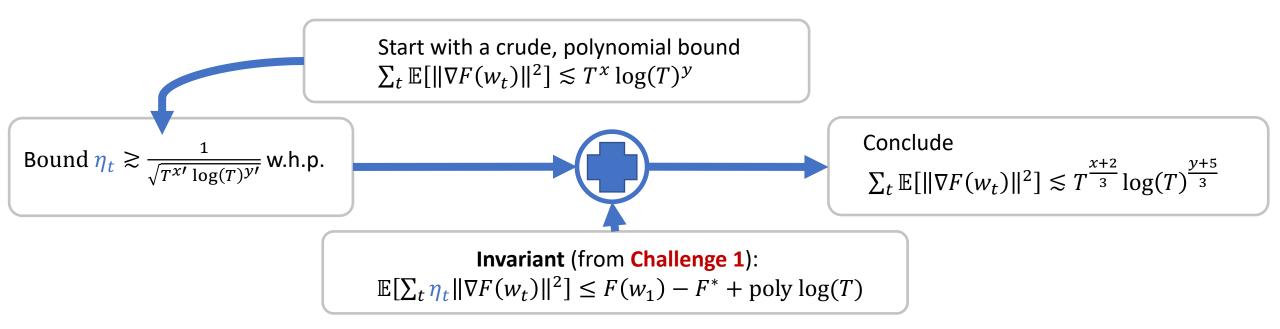
Key Idea 2: Recursively improve crude bound on $\mathbb{E}[\sum \|\nabla F(w_t)\|^2]$



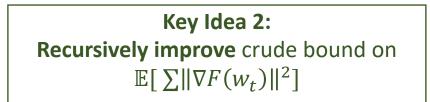
Invariant (from Challenge 1): $\mathbb{E}[\sum_t \eta_t \|\nabla F(w_t)\|^2] \le F(w_1) - F^* + \text{poly } \log(T)$

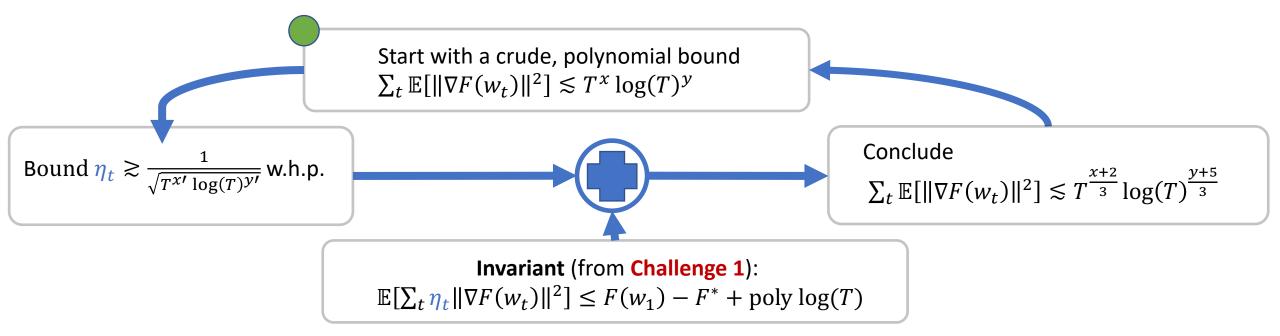
- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$



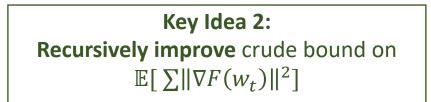


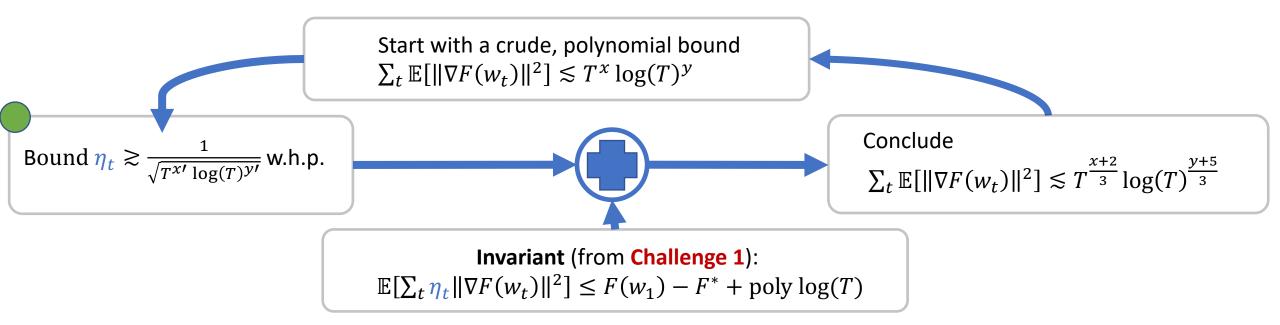
- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$



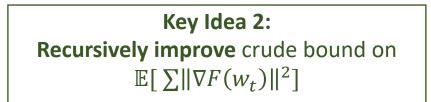


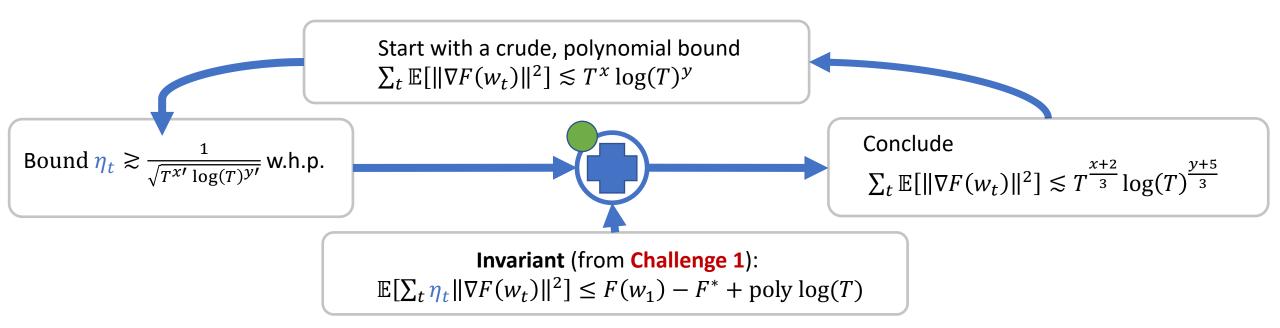
- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$



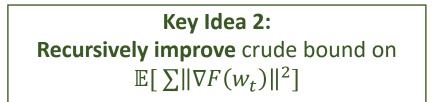


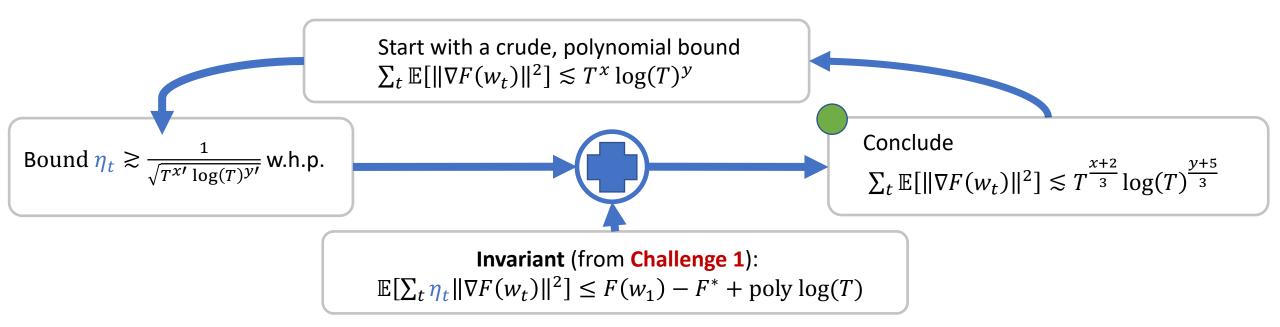
- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$



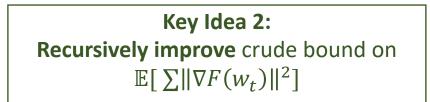


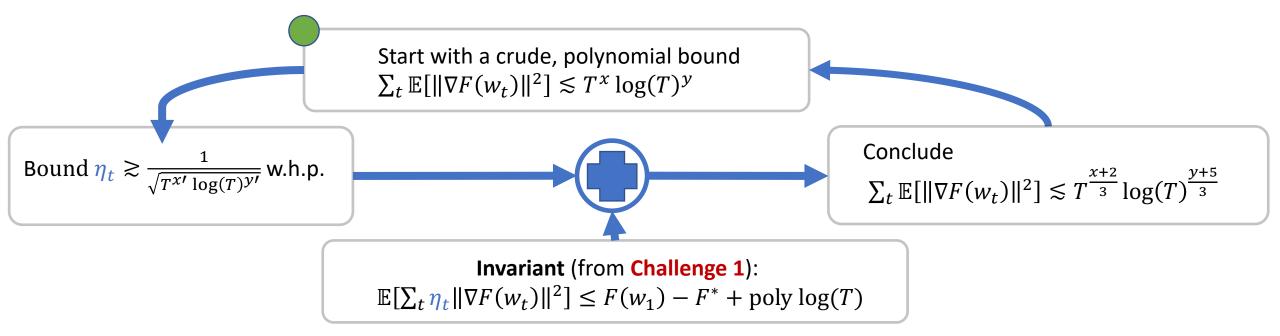
- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$





- Challenge 2: Step size scaling
 - Cannot guarantee directly that $\eta_t \gtrsim \frac{1}{\sqrt{T}}$ (even in expectation).
 - Crucial step is to bound $\mathbb{E}[\sum_t \|\nabla F(w_t)\|^2] = \tilde{O}(T).$





AdaGrad-Norm enjoys a $\min_{t} \|\nabla F(w_t)\|^2 = \tilde{O}(1/\sqrt{T})$ convergence rate in the same setting as SGD (smooth + affine).

✓ Without a uniform upper bound on the gradients or variance.

✓ For any parameter choices η , $b_0 > 0$ (no knowledge of L, σ_0 or σ_1 is required).

AdaGrad-Norm enjoys a $\min_{t} \|\nabla F(w_t)\|^2 = \tilde{O}(1/\sqrt{T})$ convergence rate in the same setting as SGD (smooth + affine).

✓ Without a uniform upper bound on the gradients or variance.

✓ For any parameter choices η , $b_0 > 0$ (no knowledge of L, σ_0 or σ_1 is required).

Remark

✓ We show that AdaGrad-Norm automatically obtains a $\tilde{O}(1/T)$ convergence rate in the small noise regime.

AdaGrad-Norm enjoys a $\min_{t} \|\nabla F(w_t)\|^2 = \tilde{O}(1/\sqrt{T})$ convergence rate in the same setting as SGD (smooth + affine).

✓ Without a uniform upper bound on the gradients or variance.

✓ For any parameter choices η , $b_0 > 0$ (no knowledge of L, σ_0 or σ_1 is required).

Remark

 \checkmark We show that AdaGrad-Norm automatically obtains a $\tilde{O}(1/T)$ convergence rate in the small noise regime.

Remark

✓ "Best of both worlds" result!

AdaGrad-Norm achieves order optimal convergence (similar to SGD) without tuning any hyperparameters!

AdaGrad-Norm enjoys a $\min_{t} \|\nabla F(w_t)\|^2 = \tilde{O}(1/\sqrt{T})$ convergence rate in the same setting as SGD (smooth + affine).

✓ Without a uniform upper bound on the gradients or variance.

✓ For any parameter choices η , $b_0 > 0$ (no knowledge of L, σ_0 or σ_1 is required).

Remark

 \checkmark We show that AdaGrad-Norm automatically obtains a $\tilde{O}(1/T)$ convergence rate in the small noise regime.

Remark

✓ "Best of both worlds" result!

AdaGrad-Norm achieves order optimal convergence (similar to SGD) without tuning any hyperparameters!

Thanks for listening!