

# Mathematics of Data: From Theory to Computation

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*Lecture 5: Optimality of Convergence rates. Accelerated Gradient/Tensor Descent Methods*

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## Recall: Gradient descent

### Problem (Unconstrained convex problem)

Consider the following convex minimization problem:

$$f^* = \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x})$$

- ▶  $f$  is a convex function that is
  - ▶ *proper* :  $\forall \mathbf{x} \in \mathbb{R}^p$ ,  $-\infty < f(\mathbf{x})$  and there exists  $\mathbf{x} \in \mathbb{R}^p$  such that  $f(\mathbf{x}) < +\infty$ .
  - ▶ *closed* : The epigraph  $\text{epi} f = \{(\mathbf{x}, t) \in \mathbb{R}^{p+1}, f(\mathbf{x}) \leq t\}$  is closed.
  - ▶ *smooth* :  $f$  is differentiable and its gradient  $\nabla f$  is  $L$ -Lipschitz.
- ▶ The solution set  $\mathcal{S}^* := \{\mathbf{x}^* \in \text{dom}(f) : f(\mathbf{x}^*) = f^*\}$  is nonempty.

### Gradient descent (GD)

Choose a starting point  $\mathbf{x}^0$  and iterate

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \nabla f(\mathbf{x}^k)$$

where  $\alpha_k$  is a step-size to be chosen so that  $\mathbf{x}^k$  converges to  $\mathbf{x}^*$ .

## Convergence rate of gradient descent

### Theorem

Let  $f$  be a twice-differentiable convex function, if

$$f \text{ is } L\text{-smooth}, \quad \alpha = \frac{1}{L} : \quad f(\mathbf{x}^k) - f(\mathbf{x}^*) \leq \frac{2L}{k+4} \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2$$

$$f \text{ is } L\text{-smooth and } \mu\text{-strongly convex}, \quad \alpha = \frac{2}{L+\mu} : \quad \|\mathbf{x}^k - \mathbf{x}^*\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^k \|\mathbf{x}^0 - \mathbf{x}^*\|_2$$

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Note that  $\frac{L-\mu}{L+\mu} = \frac{\kappa-1}{\kappa+1}$ , where  $\kappa := \frac{L}{\mu}$  is the condition number of  $\nabla^2 f$ .

## Information theoretic lower bounds [36]

**Question:**      ○ What is the **best** achievable rate for a **first-order** method?

$f \in \mathcal{F}_L^\infty$ :  $\infty$ -differentiable and  $L$ -smooth

It is possible to construct a function in  $\mathcal{F}_L^\infty$ , for which **any** first order method must satisfy

$$f(\mathbf{x}^k) - f(\mathbf{x}^*) \geq \frac{3L}{32(k+1)^2} \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2 \quad \text{for all } k \leq (p-1)/2. \quad (1)$$

$f \in \mathcal{F}_{L,\mu}^\infty$ :  $\infty$ -differentiable,  $L$ -smooth and  $\mu$ -strongly convex

It is possible to construct a function in  $\mathcal{F}_{L,\mu}^\infty$ , for which **any** first order method must satisfy

$$\|\mathbf{x}^k - \mathbf{x}^*\|_2 \geq \left( \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}} \right)^k \|\mathbf{x}^0 - \mathbf{x}^*\|_2.$$

**Observations:**      ○ Note that (1) *only* holds if  $k$  is less than  $p$ , if  $k > p$  we can do better [4]

○ Gradient descent is  $\mathcal{O}(1/k)$  for  $\mathcal{F}_L^\infty$

○ It is also slower for  $\mathcal{F}_{L,\mu}^\infty$ , hence it does not achieve the lower bounds!

# Accelerated gradient descent algorithm

## Problem

*Is it possible to design first-order methods with convergence rates matching the theoretical lower bounds?*

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Accelerated Gradient Descent (AGD) methods achieve optimal convergence rates.

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#### Accelerated Gradient algorithm for $L$ -smooth (AGD-L)

1. Set  $\mathbf{x}^0 = \mathbf{y}^0 \in \text{dom}(f)$  and  $t_0 := 1$ .
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L} \nabla f(\mathbf{y}^k) \\ t_{k+1} &= (1 + \sqrt{4t_k^2 + 1})/2 \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \frac{(t_k - 1)}{t_{k+1}} (\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

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#### Accelerated Gradient algorithm for $L$ -smooth and $\mu$ -strongly convex (AGD- $\mu L$ )

1. Choose  $\mathbf{x}^0 = \mathbf{y}^0 \in \text{dom}(f)$
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \frac{1}{L} \nabla f(\mathbf{y}^k) \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \alpha (\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

where  $\alpha = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$ .

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where  $\alpha = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}$ .

#### Remark:

- AGD is not monotone, but the cost-per-iteration is essentially the same as GD.
- The momentum  $\mathbf{x}^{k+1} - \mathbf{x}^k$  acts like an “extra-gradient.”

## Global convergence of AGD [36]

### Theorem ( $f$ is convex with Lipschitz gradient)

If  $f$  is  $L$ -smooth or  $L$ -smooth and  $\mu$ -strongly convex, the sequence  $\{\mathbf{x}^k\}_{k \geq 0}$  generated by **AGD-L** satisfies

$$f(\mathbf{x}^k) - f^* \leq \frac{4L}{(k+2)^2} \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2, \quad \forall k \geq 0. \quad (2)$$

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*AGD-L is **optimal** for  $L$ -smooth but **NOT** for  $L$ -smooth and  $\mu$ -strongly convex!*

### Theorem ( $f$ is strongly convex with Lipschitz gradient)

If  $f$  is  $L$ -smooth and  $\mu$ -strongly convex, the sequence  $\{\mathbf{x}^k\}_{k \geq 0}$  generated by **AGD- $\mu$ L** satisfies

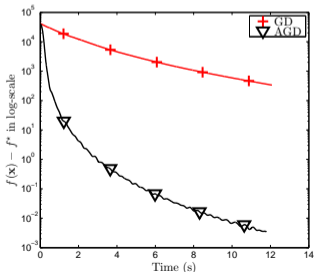
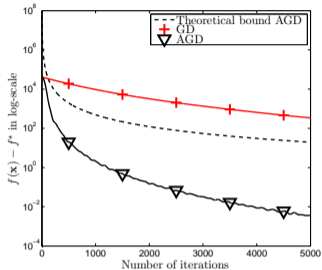
$$f(\mathbf{x}^k) - f^* \leq L \left(1 - \sqrt{\frac{\mu}{L}}\right)^k \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2, \quad \forall k \geq 0 \quad (3)$$

$$\|\mathbf{x}^k - \mathbf{x}^*\|_2 \leq \sqrt{\frac{2L}{\mu}} \left(1 - \sqrt{\frac{\mu}{L}}\right)^{\frac{k}{2}} \|\mathbf{x}^0 - \mathbf{x}^*\|_2, \quad \forall k \geq 0. \quad (4)$$

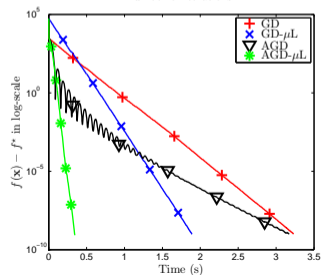
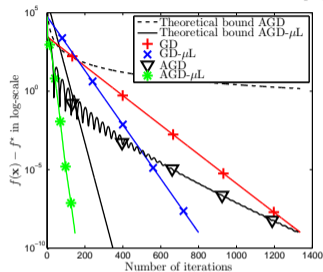
- Observations:**
- AGD-L's iterates are not guaranteed to converge in general.
  - AGD-L does not have a **linear** convergence rate for  $L$ -smooth and  $\mu$ -strongly convex.
  - AGD- $\mu$ L does, but needs to know  $\mu$ .
  - AGD achieves the iteration lowerbound within a constant!

# Example: Ridge regression

**Case 1:**  $n = 500, p = 2000, \rho = 0$

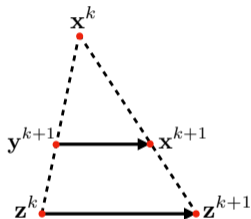


**Case 2:**  $n = 500, p = 2000, \rho = 0.01\lambda_p(\mathbf{A}^T \mathbf{A})$



## Hidden gems in AGD: The method of similar triangles

- There are several variants of Nesterov's AGD [39].



### Accelerated Gradient Descent Algorithm

- Set  $\mathbf{x}^0 = \mathbf{y}^0 = \mathbf{z}^0 \in \text{dom}(f)$  and  $t_0 := 1$ .
- For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} t^{k+1} &= \frac{2}{k+1} \\ \mathbf{y}^{k+1} &= (1 - t^{k+1})\mathbf{x}^k + t^{k+1}\mathbf{z}^k \\ \mathbf{x}^{k+1} &= \mathbf{y}^{k+1} - \frac{1}{L}\nabla f(\mathbf{y}^{k+1}) \\ \mathbf{z}^{k+1} &= \mathbf{x}^{k+1} + \left(\frac{1}{t^{k+1}} - 1\right)(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

### Remarks:

- Triangles  $(\mathbf{x}^k, \mathbf{y}^{k+1}, \mathbf{x}^{k+1})$  and  $(\mathbf{x}^k, \mathbf{z}^k, \mathbf{z}^{k+1})$  are “similar.”
- This geometric construction via averaging is typical of accelerated methods.
- Sequences  $(\mathbf{y}^{k+1}, \mathbf{z}^{k+1})$  enable acceleration by estimating a lower-bound to the problem.

## The extra-gradient algorithm

- Recall: The momentum-term  $\mathbf{x}^{k+1} - \mathbf{x}^k$  in AGD acts like an “extra-gradient.”
- However, the name extra-gradient is reserved for another algorithm approximating the proximal-point method:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \gamma \nabla f(\mathbf{x}^{k+1}) \quad (\text{PPM})$$

Extra-gradient algorithm [21]
<ol style="list-style-type: none"><li>1. Choose <math>\mathbf{x}^0 \in \text{dom}(f)</math></li><li>2. For <math>k = 0, 1, \dots</math>, iterate</li></ol> $\begin{cases} \mathbf{x}^{k+1/2} &= \mathbf{x}^k - \gamma \nabla f(\mathbf{x}^k) \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \gamma \nabla f(\mathbf{x}^{k+1/2}) \end{cases}$ <ul style="list-style-type: none"><li>▶ Pick <math>\gamma &lt; \frac{1}{L}</math>.</li><li>▶ Define <math>\bar{\mathbf{x}}^{k+1/2} = \sum_{i=1}^k \mathbf{x}^{i+1/2} / k</math></li><li>▶ <math>f(\bar{\mathbf{x}}^{k+1/2}) - f(\mathbf{x}^*) \leq O\left(\frac{1}{k}\right)</math></li></ul>

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- ▶ Pick  $\gamma < \frac{1}{L}$ .
- ▶ Define  $\bar{\mathbf{x}}^{k+1/2} = \sum_{i=1}^k \mathbf{x}^{i+1/2} / k$
- ▶  $f(\bar{\mathbf{x}}^{k+1/2}) - f(\mathbf{x}^*) \leq O\left(\frac{1}{k}\right)$

### Accelerated extra-gradient algorithm [11]

1. Set  $\mathbf{x}^0 = \mathbf{z}^0 = \mathbf{x}^0$
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{x}^{k+1/2} &= \mathbf{x}^k - \alpha_k \gamma \nabla f(\tilde{\mathbf{x}}^k) \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \gamma \nabla f(\bar{\mathbf{x}}^{k+1/2}) \end{cases}$$

- ▶ Pick  $\gamma < \frac{1}{L}$  and define  $\alpha_k = O(k)$
- ▶  $\tilde{\mathbf{x}}^k = \frac{\alpha_k \mathbf{x}^k + \sum_{i=1}^{k-1} \alpha_i \mathbf{x}^{i+1/2}}{\sum_{i=1}^k \alpha_i}$ ,  $\bar{\mathbf{x}}^{k+1/2} = \frac{\sum_{i=1}^k \alpha_i \mathbf{x}^{i+1/2}}{\sum_{i=1}^k \alpha_i}$
- ▶  $f(\bar{\mathbf{x}}^{k+1/2}) - f(\mathbf{x}^*) \leq O\left(\frac{1}{k^2}\right)$  [11]

## Gradient descent vs. Accelerated gradient descent

### Assumptions, step sizes and convergence rates

Gradient descent:

$$f \text{ is } L\text{-smooth, } \alpha = \frac{1}{L} : \quad f(\mathbf{x}^k) - f(\mathbf{x}^*) \leq \frac{2L}{k+4} \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2.$$

Accelerated Gradient Descent:

$$f \text{ is } L\text{-smooth, } \alpha = \frac{1}{L} : \quad f(\mathbf{x}^k) - f(x^*) \leq \frac{4L}{(k+2)^2} \|\mathbf{x}^0 - \mathbf{x}^*\|_2^2, \quad \forall k \geq 0.$$

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**Observations:**

- We require  $\alpha_t$  to be a function of  $L$ .
- It may not be possible to know exactly the Lipschitz constant.
- Adaptation to local geometry  $\rightarrow$  may lead to larger steps.

# Adaptive first-order methods and Newton method

## Adaptive methods

Adaptive methods converge with fast rates **without knowing** the smoothness constant.

They do so by making use of the information from **gradients and their norms**.

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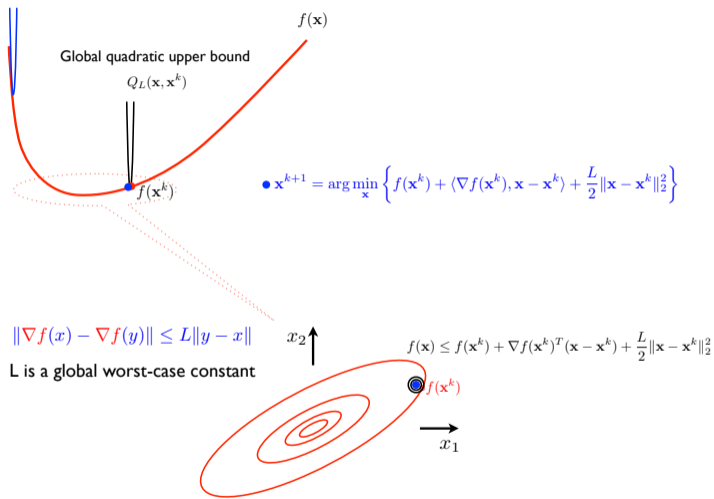
They do so by making use of the information from **gradients and their norms**.

## Newton method

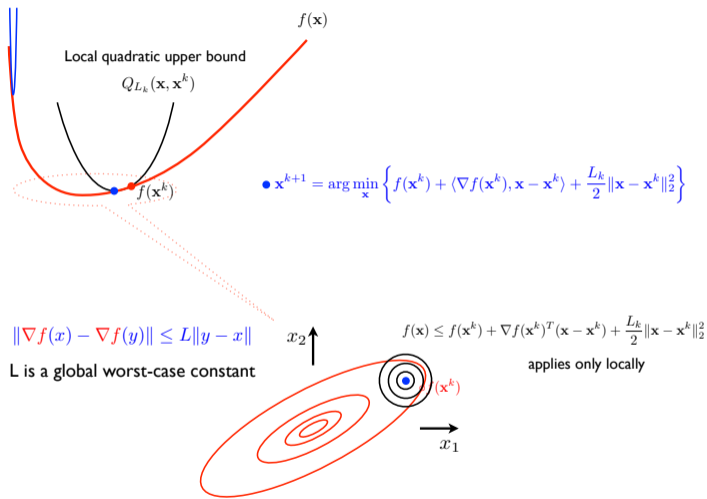
**Higher-order information**, e.g., Hessian, gives a finer characterization of local behavior.

Newton method achieves **asymptotically better** local rates, but for additional **cost**.

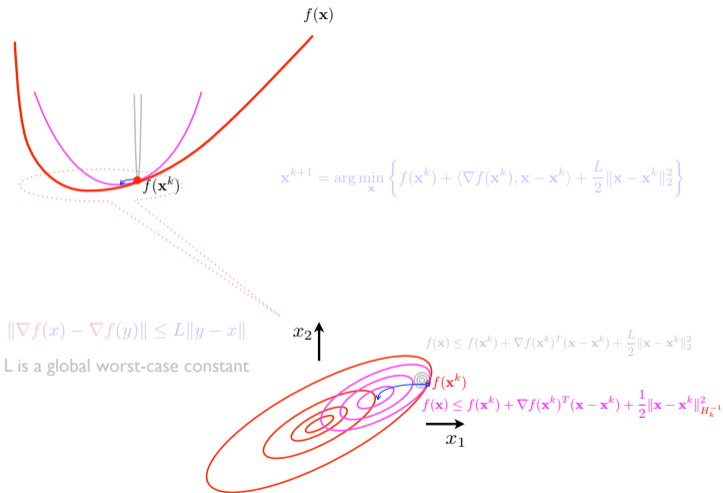
## How can we better adapt to the local geometry?



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## Variable metric gradient descent algorithm

### Variable metric gradient descent algorithm

1. Choose  $\mathbf{x}^0 \in \mathbb{R}^P$  as a starting point and  $\mathbf{H}_0 \succ 0$ .
2. For  $k = 0, 1, \dots$ , perform:

$$\begin{cases} \mathbf{d}^k & := -\mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k), \\ \mathbf{x}^{k+1} & := \mathbf{x}^k + \alpha_k \mathbf{d}^k, \end{cases}$$

where  $\alpha_k \in (0, 1]$  is a given step size.

3. Update  $\mathbf{H}_{k+1} \succ 0$  if necessary.

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### Common choices of the variable metric $\mathbf{H}_k$

- ▶  $\mathbf{H}_k := \lambda_k \mathbf{I} \implies$  gradient descent method.
- ▶  $\mathbf{H}_k := \mathbf{D}_k$  (a positive diagonal matrix)  $\implies$  adaptive gradient methods.
- ▶  $\mathbf{H}_k := \nabla^2 f(\mathbf{x}^k) \implies$  Newton method.
- ▶  $\mathbf{H}_k \approx \nabla^2 f(\mathbf{x}^k) \implies$  quasi-Newton method.

## Adaptive gradient methods

### Intuition

Adaptive gradient methods adapt locally by setting  $\mathbf{H}_k$  as a function of **past gradient information**.

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Adaptive gradient methods adapt locally by setting  $\mathbf{H}_k$  as a function of **past gradient information**.

- o Roughly speaking,  $\mathbf{H}_k = \text{function}(\nabla f(\mathbf{x}^1), \nabla f(\mathbf{x}^2), \dots, \nabla f(\mathbf{x}^k))$
- o Some well-known examples:

### AdaGrad (Scalar) [12, 32]

$$\mathbf{H}_k = \sqrt{\sum_{t=1}^k (\nabla f(\mathbf{x}^t)^\top \nabla f(\mathbf{x}^t))}$$

### \*RmsProp [51]

$$\mathbf{H}_k = \sqrt{\beta \mathbf{H}_{k-1} + (1 - \beta) \text{diag}(\nabla f(\mathbf{x}^k))^2}$$

### \*ADAM [20]

$$\begin{aligned}\hat{\mathbf{H}}_k &= \beta \hat{\mathbf{H}}_{k-1} + (1 - \beta) \text{diag}(\nabla f(\mathbf{x}^k))^2 \\ \mathbf{H}_k &= \sqrt{\hat{\mathbf{H}}_k / (1 - \beta^k)}\end{aligned}$$

## AdaGrad - Adaptive gradient method with $\mathbf{H}_k = \lambda_k \mathbf{I}$ [32]

- If  $\mathbf{H}_k = \lambda_k \mathbf{I}$ , it becomes gradient descent method with adaptive step-size  $\frac{\alpha_k}{\lambda_k}$ .

### How step-size adapts?

If gradient  $\|\nabla f(\mathbf{x}^k)\|$  is large/small  $\rightarrow$  AdaGrad adjusts step-size  $\alpha_k/\lambda_k$  smaller/larger

#### Adaptive gradient descent (AdaGrad with $\mathbf{H}_k = \lambda_k \mathbf{I}$ ) [25]

1. Set  $Q^0 = 0$ .
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} Q^k &= Q^{k-1} + \|\nabla f(\mathbf{x}^k)\|^2 \\ \mathbf{H}_k &= \sqrt{Q^k} \mathbf{I} \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) \end{cases}$$

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### Adaptation through first-order information

- ▶ When  $H_k = \lambda_k I$ , AdaGrad estimates local geometry through gradient norms.
- ▶ Akin to estimating a local quadratic upper bound (majorization / minimization) using gradient history.



## AdaGrad - Adaptive gradient method with $\mathbf{H}_k = \mathbf{D}_k$ [50]

- Suppose  $\mathbf{H}_k$  is diagonal,

$$\mathbf{H}_k := \begin{bmatrix} \lambda_{k,1} & & 0 \\ & \ddots & \\ 0 & & \lambda_{k,d} \end{bmatrix},$$

- For each coordinate  $i$ , we have different step-size  $\frac{\alpha_k}{\lambda_{k,i}}$  is the step-size.

### Adaptive gradient descent(AdaGrad with $\mathbf{H}_k = \mathbf{D}_k$ )

- Set  $\mathbf{Q}^0 = 0$ .
- For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{Q}^k &= \mathbf{Q}^{k-1} + \text{diag}(\nabla f(\mathbf{x}^k))^2 \\ \mathbf{H}_k &= \sqrt{\mathbf{Q}^k} \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) \end{cases}$$

## AdaGrad - Adaptive gradient method with $\mathbf{H}_k = \mathbf{D}_k$ [50]

- Suppose  $\mathbf{H}_k$  is diagonal,

$$\mathbf{H}_k := \begin{bmatrix} \lambda_{k,1} & & 0 \\ & \ddots & \\ 0 & & \lambda_{k,d} \end{bmatrix},$$

- For each coordinate  $i$ , we have different step-size  $\frac{\alpha_k}{\lambda_{k,i}}$  is the step-size.

### Adaptive gradient descent(AdaGrad with $\mathbf{H}_k = \mathbf{D}_k$ )

- Set  $\mathbf{Q}^0 = 0$ .
- For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{Q}^k &= \mathbf{Q}^{k-1} + \text{diag}(\nabla f(\mathbf{x}^k))^2 \\ \mathbf{H}_k &= \sqrt{\mathbf{Q}^k} \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) \end{cases}$$

### Adaptation across each coordinate

- ▶ When  $\mathbf{H}_k = \mathbf{D}_k$ , we adapt across each coordinate individually.
- ▶ Essentially, we have a finer treatment of the function we want to optimize.

## Convergence rate for AdaGrad

### Original convergence for a different function class

Consider a proper, convex function  $f$  such that it is  $G$ -Lipschitz continuous (NOT  $L$ -smooth). Let  $D = \max_k \|\mathbf{x}^k - \mathbf{x}^*\|_2$  and  $\alpha_k = \frac{D}{\sqrt{2}}$ . Define  $\bar{\mathbf{x}}^k = (\sum_{i=1}^k \mathbf{x}^i)/k$ . Then,

$$f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^*) \leq \frac{1}{k} \sqrt{2D^2 \sum_{i=1}^k \|\nabla f(\mathbf{x}^i)\|_2^2} \leq \frac{\sqrt{2}DG}{\sqrt{k}}$$

### A more familiar convergence result [25]

Assume  $f$  is  $L$ -smooth,  $D = \max_t \|\mathbf{x}^k - \mathbf{x}^*\|_2$  and  $\alpha_k = \frac{D}{\sqrt{2}}$ . Define  $\bar{\mathbf{x}}^k = (\sum_{i=1}^k \mathbf{x}^i)/k$ . Then,

$$f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^*) \leq \frac{1}{k} \sqrt{2D^2 \sum_{i=1}^k \|\nabla f(\mathbf{x}^i)\|_2^2} \leq \frac{4D^2L}{k}$$

## AcceleGrad - Adaptive gradient + Accelerated gradient [26]

### Motivation behind AcceleGrad

Is it possible to achieve acceleration for when  $f$  is  $L$ -smooth, without knowing the Lipschitz constant?

- The answer is yes! AcceleGrad combines an accelerated algorithm with AdaGrad step-size.
- A rough comparison of the accelerated methods:

#### Accelerated Gradient algorithm

1. Choose  $\mathbf{x}^0 = \mathbf{y}^0 \in \text{dom}(f)$
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{x}^{k+1} &= \mathbf{y}^k - \alpha \nabla f(\mathbf{y}^k) \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} + \gamma_{k+1}(\mathbf{x}^{k+1} - \mathbf{x}^k) \end{cases}$$

- ▶ for some proper choice of  $\alpha$  and  $\gamma_{k+1}$ .

#### AcceleGrad (Accelerated Adaptive Gradient Method)

1. Set  $\mathbf{y}^0 = \mathbf{z}^0 = \mathbf{x}^0$
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \tau_k &:= 1/\alpha_k \\ \mathbf{x}^{k+1} &= \tau_k \mathbf{z}^k + (1 - \tau_k) \mathbf{y}^k \\ \mathbf{z}^{k+1} &= \mathbf{z}^k - \alpha_k \eta_k \nabla f(\mathbf{x}^k) \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} - \eta_k \nabla f(\mathbf{x}^k) \end{cases}$$

- ▶ for  $\alpha_k = (k + 1)/4$ , and
- ▶ 
$$\eta_k = \frac{2D}{\sqrt{G^2 + \sum_{i=0}^k (\alpha_i)^2 \|\nabla f(\mathbf{x}^i)\|^2}}$$

## Convergence of AcceleGrad

### Theorem (Convergence rate of AcceleGrad)

Let the sequence  $\{\mathbf{y}^k\}$  be generated by AcceleGrad. Under the assumptions

- ▶  $f$  is convex and  $L$ -smooth,
- ▶ Iterates are bounded, such that  $D = \max_{\mathbf{x}, \mathbf{y} \in \mathbb{R}^d} \|\mathbf{x} - \mathbf{y}\|$ ,
- ▶ Gradient norms are bounded  $\|\nabla f(\mathbf{x})\| \leq G$ ,

AcceleGrad has the following guarantee:

$$f(\bar{\mathbf{y}}^k) - \min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) \leq O\left(\frac{DG + LD^2 \log(LD/G)}{k^2}\right),$$

where  $\bar{\mathbf{y}}^k = (\sum_{i=0}^{k-1} \alpha_k \mathbf{y}^{k+1}) / (\sum_{i=0}^{k-1} \alpha_k)$  is the average iterate.

- Remarks:**
- Accelegrad is a nearly “universal” algorithm (more on this later!)
  - We still need a bound on  $G$  and  $D$  to run the algorithm.
  - It cannot handle constraints.

## UniXGrad - Accelerated Extra-gradient (!) algorithm for constraints [19]

- o Universal extra-gradient method offers improvements over AcceleGrad

Extra-Gradient algorithm
<ol style="list-style-type: none"><li>1. Choose <math>\mathbf{x}^0 \in \text{dom}(f)</math></li><li>2. For <math>k = 0, 1, \dots</math>, iterate</li></ol>
$\begin{cases} \mathbf{x}^{k+1/2} &= \mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k) \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha \nabla f(\mathbf{x}^{k+1/2}) \end{cases}$

- ▶ Pick  $\alpha < 1/L$ .

UniXGrad
<ol style="list-style-type: none"><li>1. Set <math>\mathbf{x}^0 = \mathbf{z}^0 = \mathbf{x}^0</math></li><li>2. For <math>k = 0, 1, \dots</math>, iterate</li></ol>
$\begin{cases} \mathbf{x}^{k+1/2} &= \Pi_{\mathcal{X}} \left( \mathbf{x}^k - \alpha_k \eta_k \nabla f(\tilde{\mathbf{x}}^k) \right) \\ \mathbf{x}^{k+1} &= \Pi_{\mathcal{X}} \left( \mathbf{x}^k - \alpha_k \eta_k \nabla f(\bar{\mathbf{x}}^{k+1/2}) \right) \end{cases}$

- ▶  $\Pi_{\mathcal{X}}(\mathbf{x})$  is Euclidean projection onto  $\mathcal{X}$  and  $\alpha_k = k$
- ▶  $\tilde{\mathbf{x}}^k = \frac{\alpha_k \mathbf{x}^k + \sum_{i=1}^{k-1} \alpha_i \mathbf{x}^{i+1/2}}{\sum_{i=1}^k \alpha_i}$ ,  $\bar{\mathbf{x}}^{k+1/2} = \frac{\sum_{i=1}^k \alpha_i \mathbf{x}^{i+1/2}}{\sum_{i=1}^k \alpha_i}$
- ▶  $\eta_k = \frac{2D}{\sqrt{1 + \sum_{i=1}^k (\alpha_i)^2 \|\nabla f(\bar{\mathbf{x}}^{k+1/2}) - \nabla f(\tilde{\mathbf{x}}^k)\|^2}}$

# Convergence of UniXGrad

## Theorem (Convergence rate of UniXGrad)

Let the sequence  $\{\mathbf{x}^{k+1/2}\}$  be generated by UniXGrad. Under the assumptions

- ▶  $f$  is convex and  $L$ -smooth,
- ▶ Constraint set  $\mathcal{X}$  has bounded diameter, i.e.,  $D = \max_{\mathbf{x}, \mathbf{y} \in \mathcal{X}} \|\mathbf{x} - \mathbf{y}\|$ ,

UniXGrad guarantees the following:

$$f(\bar{\mathbf{x}}^{k+1/2}) - \min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}) \leq O\left(\frac{LD^2}{k^2}\right),$$

where  $\bar{\mathbf{x}}^{k+1/2} = \frac{\sum_{i=1}^k \alpha_i \mathbf{x}^{i+1/2}}{\sum_{i=1}^k \alpha_i}$  is the average iterate.

- Remarks:**
- UniXGrad is a truly “universal” algorithm (more on this later!)
  - We still need a bound on  $D$  to run the algorithm.
  - It can handle constraints.
  - It removes the log-factor in AcceleGrad.

## Adaptive methods and open questions

**Question:**      ○ Can we improve diameter  $D$  dependence on adaptive methods?

**Answer:**        ○ UnderGrad [3] has  $O(\log D)$  dependence instead of  $\mathcal{O}(D)$  while retaining the fast rates.

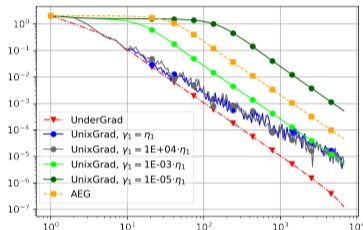


Figure: UniXGrad vs. UnderGrad vs. Accelerated extra-gradient algorithm.

**Question:**      ○ Can we go beyond  $O(1/k^2)$  rate while adapting to problem parameters and oracle noise?

**Answer:**        ○ Yes, ExtraNewton<sup>TM</sup> [2] achieves a rate of  $O\left(\frac{1}{k^3}\right)$  using a regularized Newton update.

## A quick look at descent methods: beyond first-order minimization

### Revisiting majorization-minimization

- ▶ Gradient descent, for  $\alpha > 0$ :

$$\begin{aligned}\mathbf{x}^{k+1} &= \arg \min_{\mathbf{x} \in \mathbb{R}^d} \left\{ f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{1}{2\alpha} \|\mathbf{x} - \mathbf{x}^k\|^2 \right\} \\ &= \mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k).\end{aligned}$$

- ▶ Newton's method, for  $\alpha > 0$ :

$$\begin{aligned}\mathbf{x}^{k+1} &= \arg \min_{\mathbf{x} \in \mathbb{R}^d} \left\{ f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{1}{2\alpha} \langle \nabla^2 f(\mathbf{x}^k)(\mathbf{x} - \mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle \right\} \\ &= \mathbf{x}^k - \alpha (\nabla^2 f(\mathbf{x}^k))^{-1} \nabla f(\mathbf{x}^k).\end{aligned}$$

- ▶ Regularized Newton's method, for  $\alpha, \beta > 0$  [24, 31]:

$$\begin{aligned}\mathbf{x}^{k+1} &= \arg \min_{\mathbf{x} \in \mathbb{R}^d} \left\{ f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{1}{2\alpha} \langle \nabla^2 f(\mathbf{x}^k)(\mathbf{x} - \mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{1}{2\alpha\beta} \|\mathbf{x} - \mathbf{x}^k\|^2 \right\} \\ &= \mathbf{x}^k - \alpha (\nabla^2 f(\mathbf{x}^k) + \beta \mathbb{I})^{-1} \nabla f(\mathbf{x}^k).\end{aligned}$$

## A quick look at descent methods: beyond first-order minimization

### Revisiting majorization-minimization

- ▶ Gradient descent, for  $\alpha > 0$ :

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- ▶ Regularized Newton's method, for  $\alpha, \beta > 0$  [24, 31]:

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#### Remarks:

- Global convergence of the Newton method is difficult.
- Local convergence of the Newton method using self-concordance is well-studied.
- Quasi-Newton methods that approximate the Newton method are well-studied [45].
- See advanced material at the end of the lecture.

## Sophia: Yet another second-order optimization algorithm [28]

### Sophia

1. Set  $\mathbf{x}^0 \in \text{dom}(f)$ ,  $m_0 = 0$ ,  $\mathbf{H}_{-n} = 0$ ,  $\hat{\mathbf{h}} \in \{\text{Hutchinson, GNB}\}$

2. For  $k = 0, 1, \dots$ , iterate

$$m_k = \beta_1 m_{k-1} + (1 - \beta_1) \nabla f(\mathbf{x}^k)$$

If  $k \bmod n = 0$ , do:

$$\mathbf{H}_k = \beta_2 \mathbf{H}_{k-n} + (1 - \beta_2) \hat{\mathbf{h}}(\mathbf{x}^k)$$

else:

$$\mathbf{H}_k = \mathbf{H}_{k-1}$$

$$\mathbf{x}^{k+1} = (1 - \alpha_k \lambda) \mathbf{x}^k - \alpha_k \cdot \text{clip}(m_k / \max\{\rho \cdot \mathbf{H}_k, \epsilon\}, 1)$$

### Remarks:

- More adaptive to heterogeneous curvatures than ADAM
- See the appendix for the Hessian estimators (Hutchinson, GNB)

## Convergence of Sophia

### Theorem (Convergence rate of Sophia)

Let the sequence  $\{\mathbf{x}^k\}$  be generated by Sophia. Assume the following:

- ▶  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  is a twice continuously differentiable, strictly convex function.
- ▶ There exists a constant  $R > 0$ , such that

$$\forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^d, \|\mathbf{x} - \mathbf{x}'\|_2 \leq R \implies \|\nabla^2 f(\mathbf{x}')^{-1} \nabla^2 f(\mathbf{x})\|_2 \leq 2.$$

Then, if we set  $\alpha = 1/2, \rho = \frac{R}{2\sqrt{d}}$ , Sophia guarantees the following

$$f(\mathbf{x}^T) - f(\mathbf{x}^*) \lesssim \frac{cR^2}{32d} e^{d \cdot \frac{f(\mathbf{x}^0) - \min_k f(\mathbf{x}^k)}{cR^2}} - T,$$

where  $c = \lambda_{\min}(\nabla^2 f(\mathbf{x}^*))$ .

## Learning rate scheduling

- Choosing a sequence of step sizes for an algorithm  $\{\alpha_k\}_{k=1}^T$  is a core problem in optimization.

### Definition

Learning rate scheduling incorporates two elements:

1. A **baseline** learning rate  $\alpha$ , which can be determined adaptively;
2. A **schedule** baseline multiplier, which has a predetermined sequence of values  $\{s_k\}_{k=1}^T$ .

- Example:**
- How can we incorporate a learning rate schedule into gradient descent (GD)?

#### GD with step size scheduling

1. Set  $\mathbf{x}^0 \in \text{dom}(f)$ .
2. For  $k = 0, 1, \dots$ , iterate

$$\left\{ \begin{array}{l} \mathbf{x}^{k+1} = \mathbf{x}^k - \alpha s_k \nabla f(\mathbf{x}^k) \end{array} \right.$$

## Basic forms

- The choice of schedule is empirically motivated.
- Basic examples include linear, exponential and step-ladder-like decreasing sequences [6].

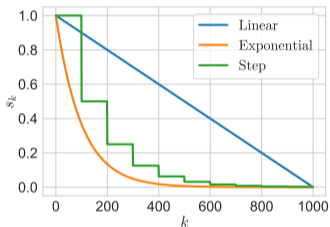


Figure: Example of common schedule (sub)sequences.

## Warm up

[15, 23] note how better results for computer vision models can be achieved by adding a *warm up* phase where the step-size scheduler initially increases the step-size multiplier from a small value to a large one.

## Additional considerations

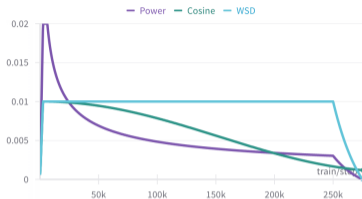


Figure: Example Warm-up+Runtime+Cool-down schedules vs. cosine annealing schedule. Credit: [48].

### Fusion of ideas

[30, 54] motivate *three-phase* schedules with results for residual neural networks and vision transformers:

1. *Warm-up* schedule with increasing step size.
2. *Runtime* schedule with constant or decreasing step size.
3. *Cool down* or *Ramp down* or *Decay* phase of sharp learning rate decrease.

#### Remarks:

- [53] theoretically motivates fast linear decay at the end of schedules.
- [18] describes the benefits of non-linear step size cool-down for language models.

## The Road Less Scheduled [9]

- o Tuning the learning rate scheduler is difficult! Can we do it without it?

ScheduleFreeGD	
<b>1.</b>	Set $\mathbf{x}^0 = \mathbf{z}^0 \in \text{dom}(f)$ and $\alpha, \beta \in [0, 1]$ .
<b>2.</b>	For $k = 0, 1, \dots$ , iterate
$\left\{ \begin{array}{l} t^{k+1} \\ \mathbf{y}^k \\ \mathbf{z}^{k+1} \\ \mathbf{x}^{k+1} \end{array} \right.$	$\left\{ \begin{array}{l} = \frac{1}{k+1} \\ = (1 - \beta)\mathbf{z}^k + \beta\mathbf{x}^k \\ = \mathbf{z}^k - \alpha\nabla f(\mathbf{y}^k) \\ = (1 - t^{k+1})\mathbf{x}^k + t^{k+1}\mathbf{z}^{k+1} \end{array} \right.$

- Remarks:**
- o This “schedule-free” algorithm uses an identical formulation to [22] up to parameter choices:
    - ▶ see Section 3 of [9]
  - o The approach differs from these conventional accelerated methods.
  - o It uses a different weight for the  $\mathbf{y}^k$  and  $\mathbf{x}^k$  interpolations:
    - ▶ constant weight  $\beta$  for  $\mathbf{y}^k$ ,
    - ▶ a decreasing weight for  $\mathbf{x}^k$  and *fixed*  $\alpha$ .

## Schedule-free theory

### Theorem (General schedule-free theory)

Let  $f$  be a convex function. Let  $\mathbf{z}^1, \dots, \mathbf{z}^T$  be arbitrary vectors and let  $w_1, \dots, w_T$  and  $\beta_1, \dots, \beta_T$  be arbitrary numbers in  $[0, 1]$ . Set:

$$\mathbf{x}^k = \frac{\sum_{i=1}^k w_i \mathbf{z}_i}{\sum_{i=1}^k w_i} = \mathbf{x}^{k-1} \underbrace{\left(1 - \frac{w_k}{\sum_{i=1}^k w_i}\right)}_{\triangleq 1-t^k} + \underbrace{\frac{w_k}{\sum_{i=1}^k w_i}}_{\triangleq t^k} \mathbf{z}^k$$
$$\mathbf{y}^k = \beta_k \mathbf{x}^k + (1 - \beta_k) \mathbf{z}^k$$

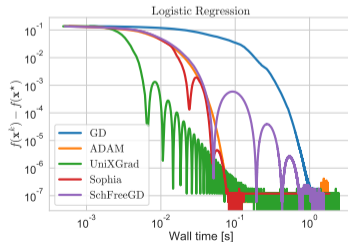
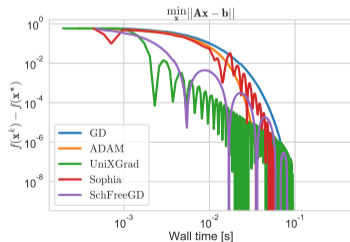
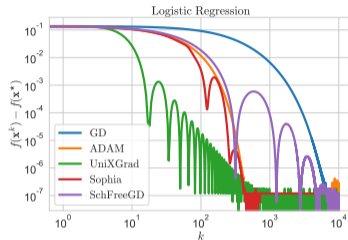
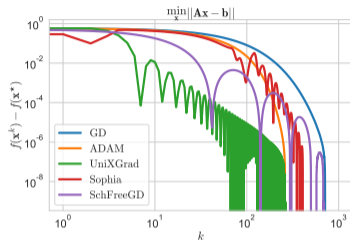
Then we have for all  $\mathbf{x}^*$ :

$$\mathbb{E}[f(\mathbf{x}^T) - f(\mathbf{x}^*)] \leq \frac{\sum_{k=1}^T w_k \mathbb{E}[\langle \nabla f(\mathbf{y}^k), \mathbf{z}^k - \mathbf{x}^* \rangle]}{\sum_{k=1}^T w_k}.$$

- Remarks:**
- The theoretical analysis is not much more involved than the adaptive methods we have seen so far!
  - We refer to the online-offline conversion in [19] and [2].
  - See the numerical evidence in the appendix.

## Example: linear and logistic regression

- Performance of adaptive algorithms on basic optimization problems



## Performance of optimization algorithms

### Time-to-reach $\epsilon$

time-to-reach  $\epsilon$  = number of iterations to reach  $\epsilon$   $\times$  per iteration time

- The **speed** of numerical solutions depends on two factors:
  - ▶ **Convergence rate** determines the number of iterations needed to obtain an  $\epsilon$ -optimal solution.
  - ▶ **Per-iteration time** depends on the information oracles, implementation, and the computational platform.
- **In general, convergence rate and per-iteration time are inversely proportional.**

Finding the **fastest** algorithm is tricky!

## Performance of optimization algorithms (convex)

A non-exhaustive comparison:

Assumptions on $f$	Algorithm	Convergence rate	Iteration complexity
$L$ -smooth	Gradient descent	Sublinear ( $1/k$ )	One gradient
	AdaGrad	Sublinear ( $1/k$ )	One gradient
	Prodigy [33]	Sublinear ( $1/k$ )	One gradient
	Accelerated GD	Sublinear ( $1/k^2$ )	One gradient
	AcceleGrad	Sublinear ( $1/k^2$ )	One gradient
	UniXGrad	Sublinear ( $1/k^2$ )	Two gradients
	Newton method	Sublinear ( $1/k$ ), Quadratic	One gradient, one linear system
	Reg. Newton method	Sublinear ( $1/k^2$ )	One gradient, one linear system
	ExtraNewton method	Sublinear ( $1/k^3$ )	Two gradients, one linear system
$L$ -smooth and $\mu$ -strongly convex	Gradient descent	Linear ( $e^{-k}$ )	One gradient
	Accelerated GD	Linear ( $e^{-k}$ )	One gradient
	Newton method	Linear ( $e^{-k}$ ), Quadratic	One gradient, one linear system
	Sophia [27]	Linear ( $e^{-k}$ )	SVD dec., one linear system, one gradient

Gradient descent:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k),$$

where the stepsize is chosen as  $\alpha \in (0, \frac{2}{L})$ .

AdaGrad:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha^k \nabla f(\mathbf{x}^k),$$

where scalar version of the step size is given by

$$\alpha^k = \frac{D}{\sqrt{\sum_{i=1}^k \|\nabla f(x^i)\|^2}}.$$

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UniXGrad:

$$\begin{aligned}\mathbf{x}^{k+1/2} &= \mathbf{x}^k - \alpha_k \eta_k \nabla f(\tilde{\mathbf{x}}^k) \\ \mathbf{x}^{k+1} &= \mathbf{x}^k + \alpha_k \eta_k \nabla f(\bar{\mathbf{x}}^{k+1/2}).\end{aligned}$$

for some proper choice of  $\alpha_k = k$  and  $\eta_k$ .

AcceleGrad:

$$\begin{aligned}\mathbf{x}^{k+1} &= \tau_k \mathbf{z}^k + (1 - \tau_k) \mathbf{y}^k \\ \mathbf{z}^{k+1} &= \mathbf{z}^k - \alpha_k \eta_k \nabla f(\mathbf{x}^k) \\ \mathbf{y}^{k+1} &= \mathbf{x}^{k+1} - \eta_k \nabla f(\mathbf{x}^k).\end{aligned}$$

for  $\alpha_k = (k+1)/4$ ,  $\tau_k = 1/\alpha_k$  and

$$\eta_k = 2D \left( G^2 + \sum_{i=0}^k (\alpha_k)^2 \|\nabla f(\mathbf{x}^i)\|^2 \right)^{-1/2}.$$

## Performance of optimization algorithms (convex)

A non-exhaustive comparison:

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	Sophia	Linear ( $e^{-k}$ )	SVD dec., one linear system, one gradient

The main computation of the Newton method requires the solution of the linear system

$$(\gamma_t \nabla^2 f(\mathbf{x}^k) + \beta_t \mathbf{I}) \mathbf{p}^k = -\nabla f(\mathbf{x}^k).$$

## Performance of optimization algorithms (convex)

A non-exhaustive comparison:

Assumptions on $f$	Algorithm	Convergence rate	Iteration complexity
$L$ -smooth	Gradient descent	Sublinear ( $1/k$ )	One gradient
	AdaGrad	Sublinear ( $1/k$ )	One gradient
	<b>Prodigy</b>	<b>Sublinear (<math>1/k</math>)</b>	<b>One gradient</b>
	Accelerated GD	Sublinear ( $1/k^2$ )	One gradient
	AcceleGrad	Sublinear ( $1/k^2$ )	One gradient
	UniXGrad	Sublinear ( $1/k^2$ )	Two gradients
	Newton method	Sublinear ( $1/k$ ), Quadratic	One gradient, one linear system
	Reg. Newton method	Sublinear ( $1/k^2$ )	One gradient, one linear system
	ExtraNewton method	Sublinear ( $1/k^3$ )	Two gradients, one linear system
$L$ -smooth and $\mu$ -strongly convex	Gradient descent	Linear ( $e^{-k}$ )	One gradient
	Accelerated GD	Linear ( $e^{-k}$ )	One gradient
	Newton method	Linear ( $e^{-k}$ ), Quadratic	One gradient, one linear system
	Sophia	Linear ( $e^{-k}$ )	SVD dec., one linear system, one gradient

Prodigy [33] is gradient descent with step sizes defined as

$$\gamma_t = \frac{d_t^2}{\sqrt{d_t^2 G^2 + \sum_{i=0}^k d_i^2 \|\nabla f(x_i)\|^2}} \quad \text{with} \quad d_{i+1} = \max \left\{ d_i, \frac{\sum_{i=0}^k \gamma_i \langle g_i, x_0 - x_i \rangle}{\|x_{i+1} - x_0\|} \right\}$$

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- Sophia stands for Second-order Clipped Stochastic Optimization [27].
- They introduce a novel Hessian estimator to stabilize the Newton's method in nonconvex landscapes.

## Overview of adaptive methods

A non-exhaustive comparison:

Assumptions on $f$	Algorithm	Convergence rate	Setting
$L$ -smooth	AdaGrad	Sublinear ( $1/k$ )	Unknown $L$
	Prodigy	Sublinear ( $1/k$ )	Unknown $\ x - x_0\ $
	AcceleGrad	Sublinear ( $1/k^2$ )	Unknown $L$
	UniXGrad	Sublinear ( $1/k^2$ )	Unknown $L$
	ExtraNewton method	Sublinear ( $1/k^3$ )	Unknown $L, \ x - x_0\ $

- Notice that  $L$  and  $\|x - x_0\|$  are rarely known in real world problems.

## The gradient method for non-convex optimization

- Remarks:**
- Gradient descent **does not** match lower bounds in **convex** setting.
  - How about non-convex problems?

### Lower bounds for non-convex problems [7]

Assume  $f$  is  $L$ -gradient Lipschitz and non-convex. Then any first-order method must satisfy,

$$\|\nabla f(\mathbf{x}^k)\|^2 = \Omega\left(\frac{1}{k}\right).$$

- Observations:**
- Gradient descent is optimal for non-convex problems, up to some constant factor!
  - Acceleration for non-convex,  $L$ -Lipschitz gradient functions is **not** as meaningful.

## Wrap up!

- The remaining slides in this lecture are advanced material.
- Lecture on Monday!

## \*Enhancements

### Two enhancements

1. Line-search for estimating  $L$  for both GD and AGD.
2. Restart strategies for AGD.

## \*Enhancements

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1. Line-search for estimating  $L$  for both GD and AGD.
2. Restart strategies for AGD.

### When do we need a line-search procedure?

We can use a line-search procedure for both GD and AGD when

- ▶  $L$  is **known** but it is **expensive to evaluate**;
- ▶ The global constant  $L$  usually **does not capture** the local behavior of  $f$  or it is **unknown**.

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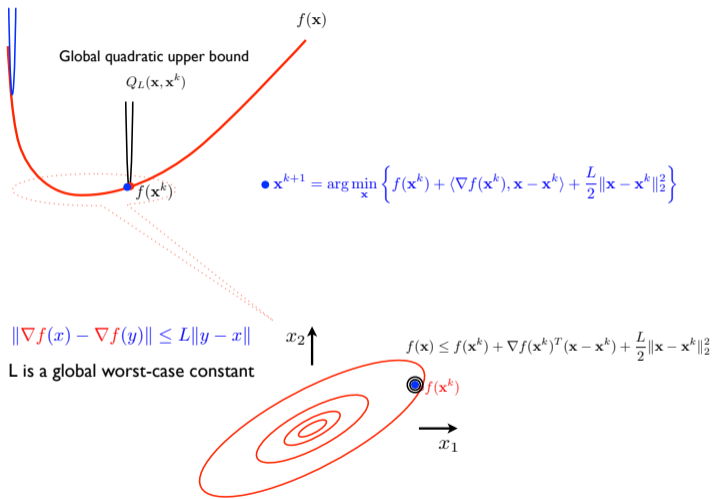
### Line-search

At each iteration, we try to find a constant  $L_k$  that satisfies:

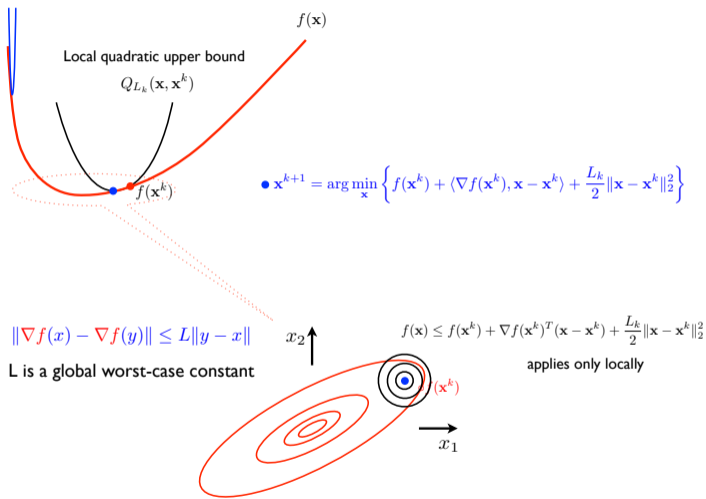
$$f(\mathbf{x}^{k+1}) \leq Q_{L_k}(\mathbf{x}^{k+1}, \mathbf{y}^k) := f(\mathbf{y}^k) + \langle \nabla f(\mathbf{y}^k), \mathbf{x}^{k+1} - \mathbf{y}^k \rangle + \frac{L_k}{2} \|\mathbf{x}^{k+1} - \mathbf{y}^k\|_2^2.$$

Here:  $L_0 > 0$  is given (e.g.,  $L_0 := c \frac{\|\nabla f(\mathbf{x}^1) - \nabla f(\mathbf{x}^0)\|_2}{\|\mathbf{x}^1 - \mathbf{x}^0\|_2}$ ) for  $c \in (0, 1]$ .

# \*How can we better adapt to the local geometry?



# \*How can we better adapt to the local geometry?



## \*Enhancements

### Why do we need a restart strategy?

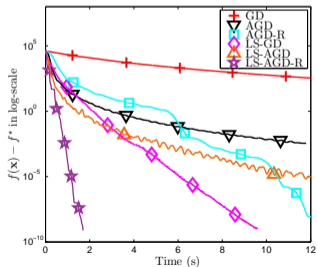
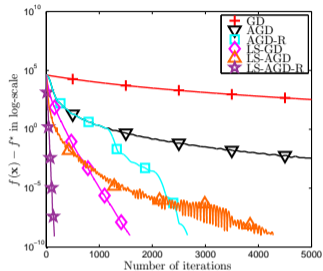
- ▶ AGD- $\mu L$  requires knowledge of  $\mu$  and AGD- $L$  does not have optimal convergence for strongly convex  $f$ .
- ▶ AGD is **non-monotonic** (i.e.,  $f(\mathbf{x}^{k+1}) \leq f(\mathbf{x}^k)$  is not always satisfied).
- ▶ AGD has a **periodic behavior**, where the **momentum** depends on the **local condition number**  $\kappa = L/\mu$ .
- ▶ A **restart strategy** tries to **reset** this **momentum** whenever we observe **high periodic behavior**. We often use function values but other strategies are possible.

### Restart strategies

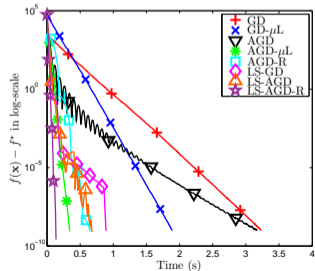
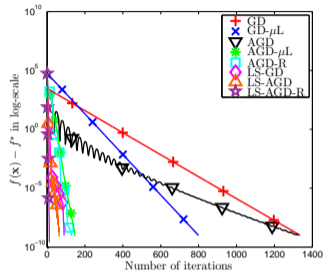
1. **O'Donoghue - Candes's strategy [42]**: There are at least **three options**: Restart with fixed number of iterations, restart based on objective values, and restart based on a gradient condition.
2. **Giselsson-Boyd's strategy [14]**: Do not require  $t_k = 1$  and do not necessary require function evaluations.
3. **Fercoq-Qu's strategy [13]**: Unconditional periodic restart for strongly convex functions. Do not require the strong convexity parameter.

# \* Example: Ridge regression

**Case 1:**  $n = 500, p = 2000, \rho = 0$



**Case 2:**  $n = 500, p = 2000, \rho = 0.01\lambda_p(\mathbf{A}^T \mathbf{A})$



## \*AcceleGrad - Adaptive gradient + Accelerated gradient [26]

### Motivation behind AcceleGrad

Is it possible to achieve acceleration when  $f$  is  $L$ -smooth, without knowing the Lipschitz constant?

<b>AcceleGrad (Accelerated Adaptive Gradient Method)</b>
<b>Input :</b> $\mathbf{x}^0 \in \mathcal{K}$ , diameter $D$ , weights $\{\eta_k\}_{k \in \mathbb{N}}$ , learning rate $\{\alpha_k\}_{k \in \mathbb{N}}$
<b>1.</b> Set $\mathbf{y}^0 = \mathbf{z}^0 = \mathbf{x}^0$ <b>2.</b> For $k = 0, 1, \dots$ , iterate $\begin{cases} \tau_k & := 1/\eta_k \\ \mathbf{x}^{k+1} & = \tau_k \mathbf{z}^k + (1 - \tau_k) \mathbf{y}^k, \text{ define } \mathbf{g}_k := \nabla f(\mathbf{x}^{k+1}) \\ \mathbf{z}^{k+1} & = \Pi_{\mathcal{K}}(\mathbf{z}^k - \eta_k \alpha_k \mathbf{g}_k) \\ \mathbf{y}^{k+1} & = \mathbf{x}^{k+1} - \alpha_k \mathbf{g}_k \end{cases}$
<b>Output :</b> $\bar{\mathbf{y}}^k \propto \sum_{i=0}^{k-1} \eta_i \mathbf{y}^{i+1}$

where  $\Pi_{\mathcal{K}}(\mathbf{y}) = \arg \min_{\mathbf{x} \in \mathcal{K}} \langle \mathbf{x} - \mathbf{y}, \mathbf{x} - \mathbf{y} \rangle$  (projection onto  $\mathcal{K}$ ).

**Remark:**      ○ This is essentially the **MD + GD** scheme [1], with an adaptive step size!

## \*AcceleGrad - Properties and convergence

### Learning rate and weight computation

Assume that function  $f$  has uniformly bounded gradient norms  $\|\nabla f(\mathbf{x}^k)\|^2 \leq G^2$ , i.e.,  $f$  is  $G$ -Lipschitz continuous. AcceleGrad uses the following weights and learning rate:

$$\eta_k = \frac{k+1}{4}, \quad \alpha_k = \frac{2D}{\sqrt{G^2 + \sum_{\tau=0}^k \alpha_{\tau}^2 \|\nabla f(\mathbf{x}_{\tau+1})\|^2}}$$

- Similar to RmsProp, AcceleGrad assigns **greater weights to recent gradients**.

### Convergence rate of AcceleGrad

Assume that  $f$  is convex and  $L$ -smooth. Let  $K$  be a convex set with bounded diameter  $D$ , and assume  $\mathbf{x}^* \in K$ . Define  $\bar{\mathbf{y}}^k = (\sum_{i=0}^{k-1} \eta_i \mathbf{y}^{i+1}) / (\sum_{i=0}^{k-1} \eta_i)$ . Then,

$$f(\bar{\mathbf{y}}^k) - \min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) \leq O\left(\frac{DG + LD^2 \log(LD/G)}{k^2}\right)$$

If  $f$  is **only** convex and  $G$ -Lipschitz, then

$$f(\bar{\mathbf{y}}^k) - \min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) \leq O\left(GD \sqrt{\log k} / \sqrt{k}\right)$$

## \*Example: Logistic regression

### Problem (Logistic regression)

Given  $\mathbf{A} \in \{0, 1\}^{n \times p}$  and  $\mathbf{b} \in \{-1, +1\}^n$ , solve:

$$f^* := \min_{\mathbf{x}, \beta} \left\{ f(\mathbf{x}) := \frac{1}{n} \sum_{j=1}^n \log \left( 1 + \exp \left( -\mathbf{b}_j (\mathbf{a}_j^T \mathbf{x} + \beta) \right) \right) \right\}.$$

### Real data

- ▶ Real data: a4a with  $\mathbf{A} \in \mathbb{R}^{n \times d}$ , where  $n = 4781$  data points,  $d = 122$  features
- ▶ All methods are run for  $T = 10000$  iterations

## \*RMSProp - Adaptive gradient method with $\mathbf{H}_k = \mathbf{D}_k$

What could be improved over AdaGrad?

1. Gradients have equal weights in step size.
2. Consider a *steep* function, flat around minimum  $\rightarrow$  slow convergence at flat region.

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#### AdaGrad with $\mathbf{H}_k = \mathbf{D}_k$

1. Set  $\mathbf{Q}_0 = 0$ .
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{Q}^k &= \mathbf{Q}^{k-1} + \text{diag}(\nabla f(\mathbf{x}^k))^2 \\ \mathbf{H}_k &= \sqrt{\mathbf{Q}^k} \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) \end{cases}$$

#### RMSProp

1. Set  $\mathbf{Q}_0 = 0$ .
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{Q}^k &= \beta \mathbf{Q}^{k-1} + (1 - \beta) \text{diag}(\nabla f(\mathbf{x}^k))^2 \\ \mathbf{H}_k &= \sqrt{\mathbf{Q}^k} \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) \end{cases}$$

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- o RMSProp uses weighted averaging with constant  $\beta$
- o Recent gradients have greater importance

## \*ADAM - Adaptive moment estimation

Over-simplified idea of ADAM

RMSProp + 2nd order moment estimation = ADAM

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ADAM	
<b>Input.</b> Step size $\alpha$ , exponential decay rates $\beta_1, \beta_2 \in [0, 1)$	
<b>1.</b> Set $\mathbf{m}_0, \mathbf{v}_0 = 0$	
<b>2.</b> For $k = 0, 1, \dots$ , iterate	
$\left\{ \begin{array}{l} \mathbf{g}_k \\ \mathbf{m}_k \\ \mathbf{v}_k \\ \hat{\mathbf{m}}_k \\ \hat{\mathbf{v}}_k \\ \mathbf{H}_k \\ \mathbf{x}^{k+1} \end{array} \right.$	$\begin{array}{l} = \nabla f(\mathbf{x}^{k-1}) \\ = \beta_1 \mathbf{m}_{k-1} + (1 - \beta_1) \mathbf{g}_k \leftarrow \text{1st order estimate} \\ = \beta_2 \mathbf{v}_{k-1} + (1 - \beta_2) \mathbf{g}_k^2 \leftarrow \text{2nd order estimate} \\ = \mathbf{m}_k / (1 - \beta_1^k) \leftarrow \text{Bias correction} \\ = \mathbf{v}_k / (1 - \beta_2^k) \leftarrow \text{Bias correction} \\ = \sqrt{\hat{\mathbf{v}}_k} + \epsilon \\ = \mathbf{x}^k - \alpha \hat{\mathbf{m}}_k / \mathbf{H}_k \end{array}$
<b>Output :</b> $\mathbf{x}^k$	

(Every vector operation is an element-wise operation)

## \*Non-convergence of ADAM and a new method: AmsGrad

- It has been shown that ADAM may not converge for *some* objective functions [44].
- An ADAM alternative is proposed that is proved to be convergent [44].

AmsGrad	
<b>Input.</b> Step size $\{\alpha_k\}_{k \in \mathbb{N}}$ , exponential decay rates $\{\beta_{1,k}\}_{k \in \mathbb{N}}$ , $\beta_2 \in [0, 1)$	
<ol style="list-style-type: none"> <li>1. Set <math>\mathbf{m}_0 = 0</math>, <math>\mathbf{v}_0 = 0</math> and <math>\hat{\mathbf{v}}_0 = 0</math></li> <li>2. For <math>k = 1, 2, \dots</math>, iterate           <math display="block">\left\{ \begin{array}{l} \mathbf{g}_k = G(\mathbf{x}^k, \theta) \\ \mathbf{m}_k = \beta_{1,k} \mathbf{m}_{k-1} + (1 - \beta_{1,k}) \mathbf{g}_k \leftarrow \text{1st order estimate} \\ \mathbf{v}_k = \beta_2 \mathbf{v}_{k-1} + (1 - \beta_2) \mathbf{g}_k^2 \leftarrow \text{2nd order estimate} \\ \hat{\mathbf{v}}_k = \max\{\hat{\mathbf{v}}_{k-1}, \mathbf{v}_k\} \text{ and } \hat{\mathbf{V}}_k = \text{diag}(\hat{\mathbf{v}}_k) \\ \mathbf{H}_k = \sqrt{\hat{\mathbf{v}}_k} \\ \mathbf{x}^{k+1} = \Pi_{\mathcal{X}}^{\sqrt{\hat{\mathbf{V}}_k}}(\mathbf{x}^k - \alpha_k \hat{\mathbf{m}}_k / \mathbf{H}_k) \end{array} \right.</math> </li> </ol>	
<b>Output :</b> $\mathbf{x}^k$	

where  $\Pi_{\mathcal{K}}^{\mathbf{A}}(\mathbf{y}) = \arg \min_{\mathbf{x} \in \mathcal{K}} \langle (\mathbf{x} - \mathbf{y}), \mathbf{A}(\mathbf{x} - \mathbf{y}) \rangle$  (weighted projection onto  $\mathcal{K}$ ).

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## The key ingredient of acceleration: (weighted) averaging

- One common theme we see in acceleration schemes is iterate averaging.
- It is important to compute averages with **larger weights on recent iterates**.
- Through UniXGrad/Extra-gradient framework, we could summarize the effect of averaging.

### Convergence rate vs. averaging parameter

Let  $\{\mathbf{x}^{k+1/2}\}$  be a sequence generated by UniXGrad algorithm, and define  $0 < \alpha_k < O(k)$  to be a non-decreasing sequence of weights. It is ensured that,

$$f(\bar{\mathbf{x}}^{k+1/2}) - \min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}) \leq O\left(\frac{1}{\sum_{i=1}^k \alpha_k}\right)$$

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#### Remarks:

- Uniform averaging:  $\alpha_k = 1 \implies O\left(\frac{1}{k}\right)$  convergence rate
- Weighted averaging:  $\alpha_k = O(k) \implies O\left(\frac{1}{k^2}\right)$  convergence rate
- In general:  $\alpha_k = O(k^p)$  for  $p \in [0, 1] \implies O\left(\frac{1}{k^{p+1}}\right)$

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$$f(\mathbf{x}^k + \mathbf{p}) \approx f(\mathbf{x}^k) + \langle \mathbf{p}, \nabla f(\mathbf{x}^k) \rangle + \frac{1}{2} \langle \mathbf{p}, \nabla^2 f(\mathbf{x}^k) \mathbf{p} \rangle$$

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- ▶ A unit step-size  $\alpha_k = 1$  can be chosen near convergence:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - (\nabla^2 f(\mathbf{x}^k))^{-1} \nabla f(\mathbf{x}^k) .$$

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### Remark

- ▶ For  $f \in \mathcal{F}_L^{2,1}$  but  $f \notin \mathcal{F}_{L,\mu}^{2,1}$ , the Hessian may not always be positive definite.

## \* (Local) Convergence of Newton method

### Lemma

Assume  $f$  is a twice differentiable convex function with minimum at  $\mathbf{x}^*$  such that:

- ▶  $\nabla^2 f(\mathbf{x}^*) \succeq \mu \mathbf{I}$  for some  $\mu > 0$ ,
- ▶  $\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\|_{2 \rightarrow 2} \leq M \|\mathbf{x} - \mathbf{y}\|_2$  for some constant  $M > 0$  and all  $\mathbf{x}, \mathbf{y} \in \text{dom}(f)$ .

Moreover, assume the starting point  $\mathbf{x}^0 \in \text{dom}(f)$  is such that  $\|\mathbf{x}^0 - \mathbf{x}^*\|_2 < \frac{2\mu}{3M}$ .

Then, the Newton method iterates converge **quadratically**:

$$\|\mathbf{x}^{k+1} - \mathbf{x}^*\| \leq \frac{M \|\mathbf{x}^k - \mathbf{x}^*\|_2^2}{2(\mu - M \|\mathbf{x}^k - \mathbf{x}^*\|_2)}.$$

### Remark

This is the fastest convergence rate we have seen so far, but it requires to solve a  $p \times p$  linear system at each iteration,  $\nabla^2 f(\mathbf{x}^k) \mathbf{p}^k = -\nabla f(\mathbf{x}^k)$ !

## \*Locally quadratic convergence of the Newton method–I

### Newton's method local quadratic convergence - Proof [41]

Since  $\nabla f(\mathbf{x}^*) = 0$  we have

$$\begin{aligned}\mathbf{x}^{k+1} - \mathbf{x}^* &= \mathbf{x}^k - \mathbf{x}^* - (\nabla^2 f(\mathbf{x}^k))^{-1} \nabla f(\mathbf{x}^k) \\ &= (\nabla^2 f(\mathbf{x}^k))^{-1} \left( \nabla^2 f(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{x}^*) - (\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^*)) \right)\end{aligned}$$

By Taylor's theorem, we also have

$$\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^*) = \int_0^1 \nabla^2 f(\mathbf{x}^k + t(\mathbf{x}^* - \mathbf{x}^k))(\mathbf{x}^k - \mathbf{x}^*) dt$$

Combining the two above, we obtain

$$\begin{aligned}& \|\nabla^2 f(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{x}^*) - (\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^*))\| \\ &= \left\| \int_0^1 (\nabla^2 f(\mathbf{x}^k) - \nabla^2 f(\mathbf{x}^k + t(\mathbf{x}^* - \mathbf{x}^k))) (\mathbf{x}^k - \mathbf{x}^*) dt \right\| \\ &\leq \int_0^1 \|\nabla^2 f(\mathbf{x}^k) - \nabla^2 f(\mathbf{x}^k + t(\mathbf{x}^* - \mathbf{x}^k))\| \|\mathbf{x}^k - \mathbf{x}^*\| dt \\ &\leq M \|\mathbf{x}^k - \mathbf{x}^*\|^2 \int_0^1 t dt = \frac{1}{2} M \|\mathbf{x}^k - \mathbf{x}^*\|^2\end{aligned}$$

## \*Locally quadratic convergence of the Newton method–II

### Newton's method local quadratic convergence - Proof [41].

- ▶ Recall

$$\mathbf{x}^{k+1} - \mathbf{x}^* = (\nabla^2 f(\mathbf{x}^k))^{-1} \left( \nabla^2 f(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{x}^*) - (\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^*)) \right)$$

$$\|\nabla^2 f(\mathbf{x}^k)(\mathbf{x}^k - \mathbf{x}^*) - (\nabla f(\mathbf{x}^k) - \nabla f(\mathbf{x}^*))\| \leq \frac{1}{2}M\|\mathbf{x}^k - \mathbf{x}^*\|^2$$

- ▶ Since  $\nabla^2 f(\mathbf{x}^*)$  is nonsingular, there must exist a radius  $r$  such that  $\|(\nabla^2 f(\mathbf{x}^k))^{-1}\| \leq 2\|(\nabla^2 f(\mathbf{x}^*))^{-1}\|$  for all  $\mathbf{x}^k$  with  $\|\mathbf{x}^k - \mathbf{x}^*\| \leq r$ .
- ▶ Substituting, we obtain

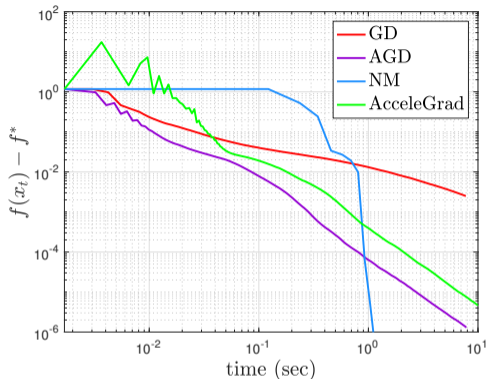
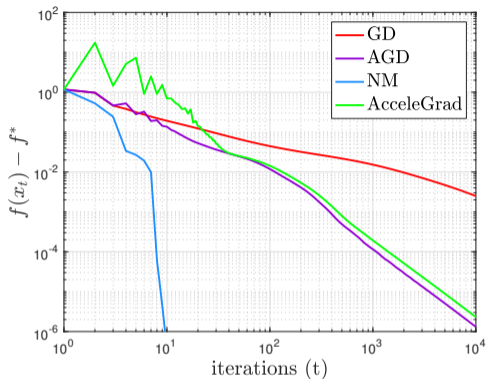
$$\|\mathbf{x}^{k+1} - \mathbf{x}^*\| \leq M\|(\nabla^2 f(\mathbf{x}^*))^{-1}\|\|\mathbf{x}^k - \mathbf{x}^*\|^2 = \tilde{M}\|\mathbf{x}^k - \mathbf{x}^*\|^2,$$

where  $\tilde{M} = M\|(\nabla^2 f(\mathbf{x}^*))^{-1}\|$ .

- ▶ If we choose  $\|\mathbf{x}^0 - \mathbf{x}^*\| \leq \min(r, 1/(2\tilde{M}))$ , we obtain by induction that the iterates  $\mathbf{x}^k$  converge quadratically to  $\mathbf{x}^*$ .

□

## \* Example: Logistic regression - GD, AGD, AcceleGrad + NM



### Parameters

- ▶ Newton's method: maximum number of iterations 30, tolerance  $10^{-6}$ .
- ▶ For GD, AGD & AcceleGrad: maximum number of iterations 10000, tolerance  $10^{-6}$ .
- ▶ Ground truth: Get a high accuracy approximation of  $x^*$  and  $f^*$  by applying Newton's method for 200 iterations.

## \* *Approximating* Hessian: Quasi-Newton methods

Quasi-Newton methods use an approximate Hessian oracle and can be more scalable.

- Useful for  $f(\mathbf{x}) := \sum_{i=1}^n f_i(\mathbf{x})$  with  $n \gg p$ .

### Main ingredients

Quasi-Newton direction:

$$\mathbf{p}^k = -\mathbf{H}_k^{-1} \nabla f(\mathbf{x}^k) = -\mathbf{B}_k \nabla f(\mathbf{x}^k).$$

- ▶ Matrix  $\mathbf{H}_k$ , or its inverse  $\mathbf{B}_k$ , undergoes low-rank updates:
  - ▶ Rank 1 or 2 updates: famous Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm.
  - ▶ Limited memory BFGS (L-BFGS).
- ▶ Line-search: The step-size  $\alpha_k$  is chosen to satisfy the **Wolfe conditions**:

$$f(\mathbf{x}^k + \alpha_k \mathbf{p}^k) \leq f(\mathbf{x}^k) + c_1 \alpha_k \langle \nabla f(\mathbf{x}^k), \mathbf{p}^k \rangle \quad (\text{sufficient decrease})$$

$$\langle \nabla f(\mathbf{x}^k + \alpha_k \mathbf{p}^k), \mathbf{p}^k \rangle \geq c_2 \langle \nabla f(\mathbf{x}^k), \mathbf{p}^k \rangle \quad (\text{curvature condition})$$

with  $0 < c_1 < c_2 < 1$ . For quasi-Newton methods, we usually use  $c_1 = 0.1$ .

- ▶ Convergence is guaranteed under the Dennis & Moré condition [10].
- ▶ For more details on quasi-Newton methods, see Nocedal&Wright's book [41].

## \*Quasi-Newton methods

### How do we update $\mathbf{B}_{k+1}$ ?

Suppose we have (note the coordinate change from  $\mathbf{p}$  to  $\bar{\mathbf{p}}$ )

$$m_{k+1}(\bar{\mathbf{p}}) := f(\mathbf{x}^{k+1}) + \langle \nabla f(\mathbf{x}^{k+1}), \bar{\mathbf{p}} - \mathbf{x}^{k+1} \rangle + \frac{1}{2} \langle \mathbf{B}_{k+1}(\bar{\mathbf{p}} - \mathbf{x}^{k+1}), (\bar{\mathbf{p}} - \mathbf{x}^{k+1}) \rangle.$$

We require the gradient of  $m_{k+1}$  to match the gradient of  $f$  at  $\mathbf{x}^k$  and  $\mathbf{x}^{k+1}$ .

- ▶  $\nabla m_{k+1}(\mathbf{x}^{k+1}) = \nabla f(\mathbf{x}^{k+1})$  as desired;
- ▶ For  $\mathbf{x}^k$ , we have

$$\nabla m_{k+1}(\mathbf{x}^k) = \nabla f(\mathbf{x}^{k+1}) + \mathbf{B}_{k+1}(\mathbf{x}^k - \mathbf{x}^{k+1})$$

which must be equal to  $\nabla f(\mathbf{x}^k)$ .

- ▶ Rearranging, we have that  $\mathbf{B}_{k+1}$  must satisfy the **secant equation**

$$\mathbf{B}_{k+1} \mathbf{s}^k = \mathbf{y}^k$$

where  $\mathbf{s}^k = \mathbf{x}^{k+1} - \mathbf{x}^k$  and  $\mathbf{y}^k = \nabla f(\mathbf{x}^{k+1}) - \nabla f(\mathbf{x}^k)$ .

- ▶ The secant equation can be satisfied with a positive definite matrix  $\mathbf{B}_{k+1}$  only if  $\langle \mathbf{s}^k, \mathbf{y}^k \rangle > 0$ , which is guaranteed to hold if the step-size  $\alpha_k$  satisfies the Wolfe conditions.

## \*Quasi-Newton methods

### BFGS method [41] (from Broyden, Fletcher, Goldfarb & Shanno)

The BFGS method arises from directly updating  $\mathbf{H}_k = \mathbf{B}_k^{-1}$ . The update on the inverse  $\mathbf{B}$  is found by solving

$$\min_{\mathbf{H}} \|\mathbf{H} - \mathbf{H}_k\|_{\mathbf{W}} \quad \text{subject to } \mathbf{H} = \mathbf{H}^T \text{ and } \mathbf{H}\mathbf{y}^k = \mathbf{s}^k \quad (5)$$

The solution is a rank-2 update of the matrix  $\mathbf{H}_k$ :

$$\mathbf{H}_{k+1} = \mathbf{V}_k^T \mathbf{H}_k \mathbf{V}_k + \eta_k \mathbf{s}^k (\mathbf{s}^k)^T ,$$

where  $\mathbf{V}_k = \mathbf{I} - \eta_k \mathbf{y}^k (\mathbf{s}^k)^T$ .

- Initialization of  $\mathbf{H}_0$  is an art. We can choose to set it to be an approximation of  $\nabla^2 f(\mathbf{x}^0)$  obtained by finite differences or just a multiple of the identity matrix.

## \*Quasi-Newton methods

### BFGS method [41] (from Broyden, Fletcher, Goldfarb & Shanno)

The BFGS method arises from directly updating  $\mathbf{H}_k = \mathbf{B}_k^{-1}$ . The update on the inverse  $\mathbf{B}$  is found by solving

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where  $\mathbf{V}_k = \mathbf{I} - \eta_k \mathbf{y}^k (\mathbf{s}^k)^T$ .

### Theorem (Convergence of BFGS)

Let  $f \in \mathcal{C}^2$ . Assume that the BFGS sequence  $\{\mathbf{x}^k\}$  converges to a point  $\mathbf{x}^*$  and  $\sum_{k=1}^{\infty} \|\mathbf{x}^k - \mathbf{x}^*\| \leq \infty$ . Assume also that  $\nabla^2 f(\mathbf{x})$  is Lipschitz continuous at  $\mathbf{x}^*$ . Then  $\mathbf{x}^k$  converges to  $\mathbf{x}^*$  at a **superlinear** rate.

### Remarks

The proof shows that given the assumptions, the BFGS updates for  $\mathbf{B}_k$  satisfy the Dennis & Moré condition, which in turn implies superlinear convergence.

## \*L-BFGS

### Challenges for BFGS

- ▶ BFGS approach stores and applies a dense  $p \times p$  matrix  $\mathbf{H}_k$ .
- ▶ When  $p$  is very large,  $\mathbf{H}_k$  can prohibitively expensive to store and apply.

### L(imited memory)-BFGS

- ▶ Do not store  $\mathbf{H}_k$ , but keep only the  $m$  most recent pairs  $\{(\mathbf{s}^i, \mathbf{y}^i)\}$ .
- ▶ Compute  $\mathbf{H}_k \nabla f(\mathbf{x}_k)$  by performing a sequence of operations with  $\mathbf{s}^i$  and  $\mathbf{y}^i$ :
  - ▶ Choose a temporary initial approximation  $\mathbf{H}_k^0$ .
  - ▶ Recursively apply  $\mathbf{H}_{k+1} = \mathbf{V}_k^T \mathbf{H}_k \mathbf{V}_k + \eta_k \mathbf{s}^k (\mathbf{s}^k)^T$ ,  $m$  times starting from  $\mathbf{H}_k^0$ :

$$\begin{aligned} \mathbf{H}_k &= \left( \mathbf{V}_{k-1}^T \cdots \mathbf{V}_{k-m}^T \right) \mathbf{H}_k^0 \left( \mathbf{V}_{k-m} \cdots \mathbf{V}_{k-1} \right) \\ &\quad + \eta_{k-m} \left( \mathbf{V}_{k-1}^T \cdots \mathbf{V}_{k-m+1}^T \right) \mathbf{s}^{k-m} (\mathbf{s}^{k-m})^T \left( \mathbf{V}_{k-m+1} \cdots \mathbf{V}_{k-1} \right) \\ &\quad + \cdots \\ &\quad + \eta_{k-1} \mathbf{s}^{k-1} (\mathbf{s}^{k-1})^T \end{aligned}$$

- ▶ From the previous expression, we can compute  $\mathbf{H}_k \nabla f(\mathbf{x}^k)$  recursively.
- ▶ Replace the oldest element in  $\{\mathbf{s}^i, \mathbf{y}^i\}$  with  $(\mathbf{s}^k, \mathbf{y}^k)$ .
- ▶ From practical experience,  $m \in (3, 50)$  does the trick.

## \*L-BFGS: A quasi-Newton method

Procedure for computing $\mathbf{H}_k \nabla f(\mathbf{x}^k)$	
0.	Recall $\eta_k = 1/\langle \mathbf{y}^k, \mathbf{s}^k \rangle$ .
1.	$\mathbf{q} = \nabla f(\mathbf{x}^k)$ .
2.	For $i = k - 1, \dots, k - m$ $\alpha_i = \eta_i \langle \mathbf{s}^i, \mathbf{q} \rangle$ $\mathbf{q} = \mathbf{q} - \alpha_i \mathbf{y}^i.$
3.	$\mathbf{r} = \mathbf{H}_k^0 \mathbf{q}$ .
4.	For $i = k - m, \dots, k - 1$ $\beta = \eta_i \langle \mathbf{y}^i, \mathbf{r} \rangle$ $\mathbf{r} = \mathbf{r} + (\alpha_i - \beta) \mathbf{s}^i.$
5.	$\mathbf{H}_k \nabla f(\mathbf{x}^k) = \mathbf{r}$ .

### Remarks

- ▶ Apart from the step  $\mathbf{r} = \mathbf{H}_k^0 \mathbf{q}$ , the algorithm requires only  $4mp$  multiplications.
- ▶ If  $\mathbf{H}_k^0$  is chosen to be diagonal, another  $p$  multiplications are needed.
- ▶ An effective initial choice is  $\mathbf{H}_k^0 = \gamma_k \mathbf{I}$ , where

$$\gamma_k = \frac{\langle \mathbf{s}^{k-1}, \mathbf{y}^{k-1} \rangle}{\langle \mathbf{y}^{k-1}, \mathbf{y}^{k-1} \rangle}$$

## \*L-BFGS: A quasi-Newton method

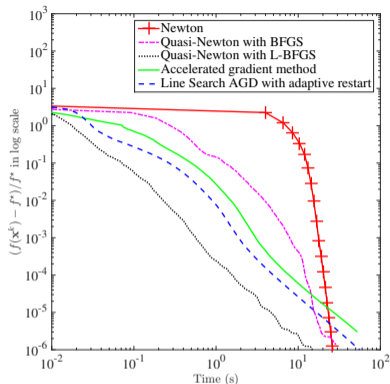
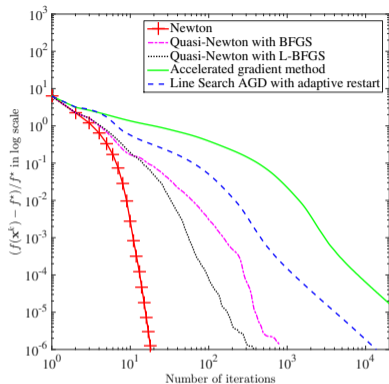
### L-BFGS

1. Choose starting point  $\mathbf{x}^0$  and  $m > 0$ .
2. For  $k = 0, 1, \dots$ 
  - 2.a Choose  $\mathbf{H}_k^0$ .
  - 2.b Compute  $\mathbf{p}^k = -\mathbf{H}_k \nabla f(\mathbf{x}^k)$  using the previous algorithm.
  - 2.c Set  $\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha_k \mathbf{p}^k$ , where  $\alpha_k$  satisfies the Wolfe conditions.  
if  $k > m$ , discard the pair  $\{\mathbf{s}^{k-m}, \mathbf{p}^{k-m}\}$  from storage.
  - 2.d Compute and store  $\mathbf{s}^k = \mathbf{x}^{k+1} - \mathbf{x}^k$ ,  $\mathbf{y}^k = \nabla f(\mathbf{x}^{k+1}) - \nabla f(\mathbf{x}^k)$ .

### Warning

L-BFGS updates does not guarantee positive semidefiniteness of the variable metric  $\mathbf{H}_k$  in contrast to BFGS.

## \* Example: Logistic regression - numerical results



### Parameters

- ▶ For BFGS, L-BFGS and Newton's method: maximum number of iterations 200, tolerance  $10^{-6}$ . L-BFGS memory  $m = 50$ .
- ▶ For accelerated gradient method: maximum number of iterations 20000, tolerance  $10^{-6}$ .
- ▶ Ground truth: Get a high accuracy approximation of  $\mathbf{x}^*$ ,  $f^*$  by running Newton's method for 200 iterations.

## \*ExtraNewton: Adaptive Newton's method with fast rates

**Question:**      ○ Under what minimal regularity conditions, can we achieve faster rates beyond  $O(1/k^2)$ ?

**Answer:**        ○ Higher-order smoothness

### Second-order smoothness

If the objective  $f$  has  $L$ -Lipschitz continuous **Hessian**, then

$$\left| f(\mathbf{x}) - f(\mathbf{y}) - \langle \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle - \frac{1}{2} \langle \nabla^2 f(\mathbf{y})(\mathbf{x} - \mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \right| \leq \frac{L}{6} \|\mathbf{x} - \mathbf{y}\|^3$$

**Question:**      ○ How can we exploit the higher-order smoothness?

**Answer:**        ○ Proximal Point method (PPM) + Newton-type updates!

## \* Better approximation, better rates

- o The extra-gradient method approximates PPM through the “extrapolation” sequence  $\mathbf{x}^{k+1/2}$  [34]

### Higher-order information for better approximation

- ▶ Extra-gradient approximates the “next” iterate,  $\mathbf{x}^{k+1}$ , using first-order information.
- ▶ Can we achieve a better estimate  $\mathbf{x}^{k+1/2}$  using second-order information? **YES!**

#### ExtraNewton [2]

1. Set  $\mathbf{x}^0 = \mathbf{z}^0 = \mathbf{x}^0$ . Define  $\alpha_k = k^2$  and  $A_k = \sum_{i=1}^k \alpha_k$
2. For  $k = 0, 1, \dots$ , iterate

$$\begin{cases} \mathbf{x}^{k+1/2} &= \mathbf{x}^k - \alpha_k \eta_k \left( \eta_k \frac{\alpha_k^2}{A_k} \nabla^2 f(\tilde{\mathbf{x}}^k) + \mathbf{I} \right)^{-1} \nabla f(\tilde{\mathbf{x}}^k) \\ \mathbf{x}^{k+1} &= \mathbf{x}^k - \alpha_k \eta_k \nabla f(\tilde{\mathbf{x}}^{k+1/2}) \end{cases}$$

$$\blacktriangleright \tilde{\mathbf{x}}^k = \frac{\alpha_k \mathbf{x}^k + \sum_{i=1}^{k-1} \alpha_i \mathbf{x}^{i+1/2}}{\sum_{i=1}^k \alpha_i}, \quad \bar{\mathbf{x}}^{k+1/2} = \frac{\sum_{i=1}^k \alpha_i \mathbf{x}^{i+1/2}}{\sum_{i=1}^k \alpha_i},$$

$$\blacktriangleright \eta_k = \frac{\gamma}{\sqrt{1 + \sum_{i=1}^{k-1} (\alpha_k)^2 \|\nabla f(\bar{\mathbf{x}}^{k+1/2}) - \nabla f(\tilde{\mathbf{x}}^k) - \nabla^2 f(\tilde{\mathbf{x}}^k)(\bar{\mathbf{x}}^{k+1/2} - \tilde{\mathbf{x}}^k)\|^2}}.$$

## \*Convergence of ExtraNewton

### Theorem ([2])

Let the sequence  $\mathbf{x}^{k+1/2}$  be generated by ExtraNewton. Under the assumptions

- ▶  $f$  has  $L$ -Lipschitz Hessian (not Lipschitz smooth),
- ▶  $D = \max_{\mathbf{x}, \mathbf{y} \in \mathcal{X}} \|\mathbf{x} - \mathbf{y}\|$

ExtraNewton guarantees that

$$f(\bar{\mathbf{x}}^{k+1/2}) - \min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}) \leq O\left(\frac{L\left(\frac{D^4}{\gamma} + D\gamma^2\right)}{k^3}\right),$$

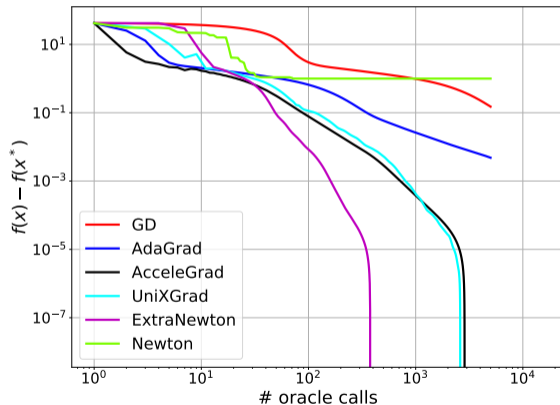
where  $\bar{\mathbf{x}}^{k+1/2} = \frac{\sum_{i=1}^k \alpha_i \mathbf{x}^{i+1/2}}{\sum_{i=1}^k \alpha_i}$  is the average sequence.

#### Remarks:

- The first globally convergent Newton method without a line-search procedure.
- The algorithm does not need to know the diameter  $D$ .
- ExtraNewton is also noise-adaptive; continuously adapts to noise in oracles.

## \*Logistic regression: ExtraNewton vs. adaptive first-order methods

- o Logistic regression with regularization using a1a dataset.
- o Comparison against first-order adaptive methods.



## \*Lower bounds for higher-order smoothness?

- Higher-order methods and the limits of their performance has received great attention lately.
- Beyond Lipschitz smoothness, we can achieve improving sublinear rates.

### Theorem ([40])

Consider that  $f$  is  $p$ -th order smooth (equivalently has Lipschitz continuous  $p + 1$ -th order derivative). Let  $\mathbf{x}^k$  be generated by some  $p$ -th order iterative tensor method. Then, it holds that

$$\min_{0 \leq i \leq k} f(\mathbf{x}^i) - \min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) = \Omega \left( \frac{1}{k^{\frac{3p+1}{2}}} \right).$$

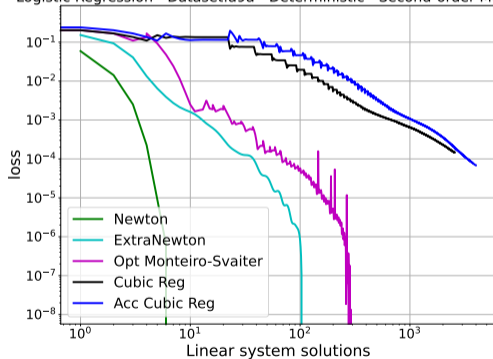
### Remarks:

- AGD matches the lower bound for 1-st order smooth function.
- The lower bound for second-order methods evaluates to  $O\left(\frac{1}{k^{7/2}}\right)$ .
- Monteiro-Svaiter's accelerated Newton method [35] and a recent work [8] archive this rate.
- In practice, all of them seem slower than ExtraNewton.

## \*Logistic regression: ExtraNewton vs. second-order methods

- Logistic regression with regularization using a9a dataset.
- Comparison against second-order methods with matching and optimal rates.

Logistic Regression - Dataset:a9a - Deterministic - Second-order Methods



- Legend:
  - ▶ Optimal Monteiro-Svaiter [8],
  - ▶ Cubic regularization of Newton's method [38],
  - ▶ Accelerated cubic regularization of Newton's methods [37].

## \*Efficient Hessian estimation for Sophia

- Sophia uses a diagonal Hessian pre-conditioner, which directly adjusts the update size of different parameters according to their curvatures.
- To mitigate the overhead, it only estimates the Hessian every  $n$  steps (unlike e.g. AdaGrad where it is done every step).
- Two efficient diagonal Hessian estimators:

Hutchinson( $\mathbf{x}$ ) [17, 46, 52]
<ol style="list-style-type: none"><li>1. Draw <math>u</math> from <math>\mathcal{N}(0, I_d)</math></li><li>2. Output <math>u \odot \nabla(\langle \nabla f(\mathbf{x}), u \rangle)</math></li></ol>



Gauss-Newton-Bartlett( $\mathbf{x}$ ) [43, 47, 5]
<ol style="list-style-type: none"><li>1. Draw a mini-batch of input <math>\{\mathbf{a}_i\}_{i=1}^B</math></li><li>2. Sample <math>\hat{b}_i \sim \text{softmax}(h_{\mathbf{x}}(\mathbf{a}_i)), \forall i \in [B]</math></li><li>3. Calculate <math>\hat{g} = \nabla(1/B \sum_{i=1}^B L(h_{\mathbf{x}}(\mathbf{a}_i), \hat{b}_i))</math></li><li>4. Output <math>B \cdot \hat{g} \odot \hat{g}</math></li></ol>



### Remarks:

- Hutchinson's estimator is unbiased and does not assume any structure of the loss, but requires Hessian-vector products
- The G.N.B. estimator always gives a positive semi-definite diagonal Hessian estimate

## \* Examples of step size schedulers with details and applications

- Common scheduler formulas used to define the warm-up, runtime or decay phase:
  - **Linear** scheduler:  $s_k = \left[ \left(1 - \frac{k}{T}\right) c_{\text{start}} + \frac{k}{T} c_{\text{end}} \right]$ , where  $c_{\text{start}}, c_{\text{end}} > 0$
  - **Exponential** scheduler:  $s_k = \gamma^k$ , where  $\gamma > 0$
  - **Step** scheduler:  $s_k = \gamma^{\lfloor \frac{k}{\tau} \rfloor}$ , where  $\gamma, \tau > 0$
- **Constant** (simplest two-phase) scheduler:  $s_k = \begin{cases} c, & \text{if } k \geq k_{\text{min}} \\ 1, & \text{otherwise} \end{cases}$ , where  $k_{\text{min}}, c > 0$
- **Cosine annealing** scheduler [29]:  $\alpha_k = \alpha_T + \frac{\alpha_0 - \alpha_T}{2} \left(1 + \cos\left(\frac{k}{T}\pi\right)\right)$ , where  $0 < \alpha_T < \alpha_0$
- **Cyclical** scheduler [49] - multiple cycles of warm-up then decay, common in deep computer vision models and adversarial training research
- **WSD** [16], **Power** [48] schedulers - three-phase step size sequences powerful in LLM pre-training

# ScheduleFree numerical evidence

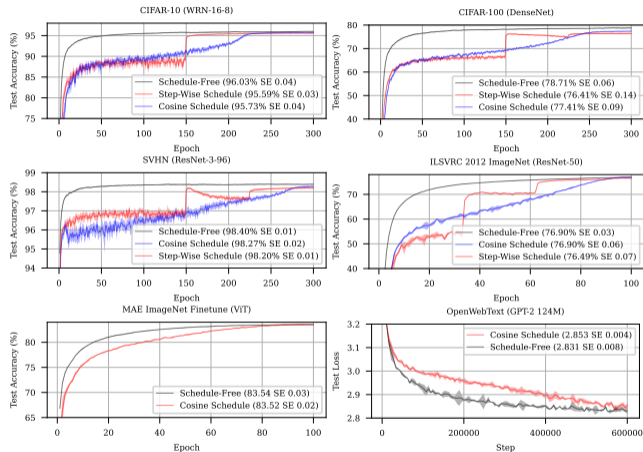


Figure: ScheduleFree experiments. Credit: [9].

## \*Tensor methods I

- Let us investigate a generic method for handling  $p$ -th order smooth problems using  $p$ -th order derivatives.

### Taylor polynomial

Let us focus on the Taylor polynomial expansion for a function  $f(\mathbf{x})$  of order  $p$  at  $\mathbf{x}$ :

$$T_p(\mathbf{x}; \mathbf{y}) = f(\mathbf{x}) + \sum_{i=1}^p \frac{1}{i!} D^i f(\mathbf{x})[\mathbf{y} - \mathbf{x}]^i,$$

- ▶  $D^i f(\mathbf{x})[h]^i$  is the directional derivative along  $h$  such that

$$D^1 f(\mathbf{x})[h] = \langle \nabla f(\mathbf{x}), h \rangle, \quad \text{and} \quad D^2 f(\mathbf{x})[h]^2 = \langle \nabla^2 f(\mathbf{x})h, h \rangle,$$

- ▶  $p$ -th order smoothness:

$$|f(\mathbf{y}) - T_p(\mathbf{x}, \mathbf{y})| \leq \frac{L_p}{(p+1)!} \|\mathbf{x} - \mathbf{y}\|^{p+1},$$

- ▶ Regularized Taylor polynomial of order  $p$  at  $\mathbf{x}$ :

$$\hat{T}_{p,H}(\mathbf{x}; \mathbf{y}) = f(\mathbf{x}) + \sum_{i=1}^p \frac{1}{i!} D^i f(\mathbf{x})[\mathbf{y} - \mathbf{x}]^i + \frac{pH}{(p+1)!} \|\mathbf{x} - \mathbf{x}^k\|^{p+1}.$$

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$$|f(\mathbf{y}) - T_p(\mathbf{x}, \mathbf{y})| \leq \frac{L_p}{(p+1)!} \|\mathbf{x} - \mathbf{y}\|^{p+1},$$

- ▶ Regularized Taylor polynomial of order  $p$  at  $\mathbf{x}$ :

$$\hat{T}_{p,H}(\mathbf{x}; \mathbf{y}) = f(\mathbf{x}) + \sum_{i=1}^p \frac{1}{i!} D^i f(\mathbf{x})[\mathbf{y} - \mathbf{x}]^i + \frac{pH}{(p+1)!} \|\mathbf{x} - \mathbf{x}^k\|^{p+1}.$$

**Remark:** ○ If  $H \geq L_p$ , then,  $f(\mathbf{y}) \leq \hat{T}_p(\mathbf{x}; \mathbf{y})$  and  $\hat{T}_p(\mathbf{x}; \mathbf{y})$  is convex. We will assume this condition!

## \*Tensor methods II

○ Recall regularized Taylor polynomial of order  $p$  at  $\mathbf{x}^k$ :

$$\hat{T}_{p,H}(\mathbf{x}; \mathbf{y}) = f(\mathbf{x}) + \sum_{i=1}^p \frac{1}{i!} D^i f(\mathbf{x}) [\mathbf{y} - \mathbf{x}]^i + \frac{pH}{(p+1)!} \|\mathbf{x} - \mathbf{x}^k\|^{p+1}.$$

**Approach:** ○ Use  $\hat{T}_{p,H}(\mathbf{x}^k; \mathbf{x})$  as the new majorizer, and minimize to obtain  $\mathbf{x}^{k+1}$

### Tensor method [40]

1. Choose  $\mathbf{x}^0 = \mathbf{y}^0 \in \text{dom}(f)$
2. For  $k = 0, 1, \dots$ , iterate
$$\left\{ \begin{array}{l} \mathbf{x}^{k+1} = \arg \min_{\mathbf{x} \in \mathbb{R}^d} \hat{T}_{p,H}(\mathbf{x}^k; \mathbf{x}) \end{array} \right.$$

### Theorem (Convergence of $p$ -th order tensor method [40])

Consider  $f$  to be  $p$ -th order smooth and let  $\{\mathbf{x}^k\}$  be generated by the Tensor method. Then, it holds that

$$f(\mathbf{x}^k) - \min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) \leq O\left(\frac{1}{t^p}\right).$$

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