#### **Inequalities** Optimization for Data Science Yilei Tu, Page 1 of 14

#### 1. Introduction Miscellaneous • $\forall x \in \mathbb{R}, 1 + x \le e^x$

# • Cosine Thm: $2\mathbf{v}^{\top}\mathbf{w} = ||\mathbf{v}||^2 + ||\mathbf{w}||^2 - ||\mathbf{v} - \mathbf{w}||^2$

For a random vector  $\mathbf{X}$ ,  $Var(\mathbf{X})$ 

• For a random vector 
$$\mathbf{X}$$
,  $\operatorname{Var}(\mathbf{X})$   
 $\mathbb{E}[\|\mathbf{X} - \mathbb{E}(\mathbf{X})\|^2] = \mathbb{E}[\|\mathbf{X}\|^2] - \|\mathbb{E}[\mathbf{X}]\|^2$ 

$$\mathbb{E}\left[\|\mathbf{X} - \mathbb{E}(\mathbf{X})\|^2\right] \le \mathbb{E}\left[\|\mathbf{X}\|^2\right]$$
•  $\sum_{t=1}^{T} 1/\sqrt{t} = \mathcal{O}(\sqrt{T})$ 

• 
$$\sum_{t=1}^{T} 1/t = \mathcal{O}(\ln T)$$
  
Eigendecomposition

• Square 
$$n \times n$$
 matrix **A**.  $\mathbf{A}\mathbf{v} = \lambda \mathbf{v}$ 

• Equation for eigenvalues: 
$$p(\lambda)$$

• Equation for eigenvalues: 
$$p(\lambda) = \det(\mathbf{A} - \lambda \mathbf{I}) = 0$$

ble and its inverse is given by 
$$A^{-1} = Q\Lambda^{-1}Q^{-1}$$

• 
$$A^n = Q\Lambda^n Q^{-1}$$
,  $A^{-1} = Q\Lambda^{-1} Q^{-1}$ 

• For every 
$$n \times n$$
 real symmetric matrix,  $\mathbf{A} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^{\mathsf{T}}$ ,

$$\mathbf{V}\mathbf{V}^{\top} = \mathbf{V}^{\top}\mathbf{V} = \mathbf{I}_{n}, \mathbf{V}^{\top} = \mathbf{V}^{-1}$$
• Can be written as  $\mathbf{A} = \sum_{i=1}^{n} \lambda_{i} \mathbf{v}_{i}, \mathbf{v}_{i}^{\top}, \{\mathbf{v}_{i}\}_{i=1}^{n} \text{ is a } \text{ For } p \geq 1 \text{ and } 1/p + 1/q = 1, \text{ havin of } \mathbb{R}^{n}$ 

• Any vector 
$$x \in \mathbb{R}^n$$
 can be written as  $\mathbf{x} = \sum_{i=1}^n \alpha_i \mathbf{v}_i$  for a unique set of  $\{\alpha_i\}_{i=1}^n$ . Then  $\mathbf{A}\mathbf{x} = \sum_{i=1}^n \lambda_i \alpha_i v_i$ ,  $\mathbf{x}^\top \mathbf{A}\mathbf{x} = \sum_{i=1}^n \alpha_i^2 \lambda_i$ 

• 
$$\max_{\|\mathbf{x}\|=1} \mathbf{x}^{\top} \mathbf{A} \mathbf{x} = \max_{i=1,\dots,n} \{\lambda_i\}, \min_{\|\mathbf{x}\|=1} \mathbf{x}^{\top} \mathbf{A} \mathbf{x} = \min_{i=1,\dots,n} \{\lambda_i\}$$

# • $\mathbf{A}^k = \sum_{i=1}^n \lambda_i^k \mathbf{v}_i \mathbf{v}_i^{\mathsf{T}}, \mathbf{A}^{-1} = \sum_{i=1}^n \lambda_i^{-1} \mathbf{v}_i \mathbf{v}_i^{\mathsf{T}}$

# Spectral Norm

# The spectral norm of a matrix A is the largest sin-

gular value of A (i.e., the square root of the largest eigenvalue of the matrix A\* A, where A\* denotes the conjugate transpose A):

$$\|\mathbf{A}\|_2 = \sqrt{\lambda_{\max}(\mathbf{A}^*\mathbf{A})} = \sigma_{\max}(\mathbf{A})$$

For the square matrix,

$$\|\mathbf{A}\|_2 := \max_{\mathbf{v} \in \mathbb{R}^d, \mathbf{v} \neq 0} \frac{\|\mathbf{A}\mathbf{v}\|}{\|\mathbf{v}\|} = \max_{\|\mathbf{v}\| = 1} \|\mathbf{A}\mathbf{v}\| = \lambda_{\max}(\mathbf{A})$$

# **Frobenius Norm**

$$\|\mathbf{A}\|_{\mathrm{F}} = \sqrt{\sum_{i,j=1}^{n} |a_{ij}|^2} = \sqrt{\operatorname{tr}(\mathbf{A}^{\top}\mathbf{A})} = \sqrt{\sum_{i=1}^{\min\{m,n\}} \sigma_i^2(\mathbf{A})}$$

•  $\|\mathbf{A}\|_2 \le \|\mathbf{A}\|_F$  for every matrix (Proof see Hw8) •  $\|\mathbf{A}\mathbf{y}\|_{2} \le \|\mathbf{A}\|_{2} \cdot \|\mathbf{y}\|_{2}$  for any  $\mathbf{A}, \mathbf{y}$ 

• 
$$\|\mathbf{A}\mathbf{x}\|_2^2 \le \lambda_{\max}(\mathbf{A}) \cdot \mathbf{x}^\top \mathbf{A}\mathbf{x} = \|\mathbf{A}\|_2 \cdot \mathbf{x}^\top \mathbf{A}\mathbf{x}$$
  
•  $\|\mathbf{A}\mathbf{x}\|_2^2 \ge \lambda_{\min}^2(\mathbf{A}) \cdot \|\mathbf{x}\|_2^2$ 

• 
$$\lambda_{\min}(\mathbf{A}) \cdot \|\mathbf{x}\|_2^2 \le \mathbf{x}^\top \mathbf{A} \mathbf{x} \le \lambda_{\max}(\mathbf{A}) \cdot \|\mathbf{x}\|_2^2 = \|\mathbf{A}\| \|\mathbf{x}\|_2^2$$

• If 
$$\lambda_{\min}(\mathbf{A}) \geq \mu$$
 and/or  $\lambda_{\max}(\mathbf{A}) \leq L$ , then  $\lambda_{\max}(\mathbf{A}^{-1}) \leq \frac{1}{\mu}$  and/or  $\lambda_{\min}(\mathbf{A}^{-1}) \leq \frac{1}{L}$ 

#### **General Norms and Dual Norms** Norm

A function  $\|\cdot\|: \mathbb{R}^d \to \mathbb{R}_+$  is a norm if (a)  $\|\mathbf{x}\| = 0$  if and only if  $\mathbf{x} = 0$ ; (b)  $\|\alpha \mathbf{x}\| = |\alpha| \cdot \|\mathbf{x}\|$ ; (c)  $||\mathbf{x} + \mathbf{y}|| \le ||\mathbf{x}|| + ||\mathbf{y}||$ . **Dual Norm** 

$$\|\mathbf{y}\|_* := \max_{\|\mathbf{x}\| \le 1} \langle \mathbf{x}, \mathbf{y} \rangle$$
  
 \ge 1 and  $1/p + 1/q = 1$ ,

$$\|\mathbf{x}\|_p := \left(\sum_{i=1}^d |x_i|^p\right)^{1/p}, \|\cdot\|_{p,*} = \|\cdot\|_q$$

# **General Smoothness and Strong Convexity**

Convexity:

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x})$$

Inequality:  $\frac{1}{\sqrt{d}} \|\mathbf{x}\|_2 \le \|\mathbf{x}\|_{\infty} \le \|\mathbf{x}\|_2 \le \|\mathbf{x}\|_1 \le \sqrt{d} \|\mathbf{x}\|_2$ 

• Optimality Condition for Convex Functions: Suppose that  $f: dom(f) \to \mathbb{R}$  is convex and differentiable over an open domain  $dom(f) \subseteq \mathbb{R}^d$ , and let  $X \subseteq \text{dom}(f)$  be a convex set. Point  $\mathbf{x}^* \in X$  is a minimizer of  $\hat{f}$  over X iff

$$\nabla f(\mathbf{x}^*)^{\top} (\mathbf{x} - \mathbf{x}^*) \ge 0 \quad \forall \mathbf{x} \in X$$

#### • Lipschitz continuity: $f(\mathbf{x})$ is B-Lipschitz continuous on X if

 $||f(\mathbf{x}) - f(\mathbf{y})| \le B||\mathbf{x} - \mathbf{y}||_{\bullet}, \forall \mathbf{x}, \mathbf{y} \in X$  $\iff$   $\|\mathbf{g}\|_* \leq B \text{ for all } \mathbf{g} \in \partial f(\mathbf{x})$ 

In particular,  $||f(\mathbf{x}) - f(\mathbf{y})||_2 \le B||\mathbf{x} - \mathbf{y}||_2 \iff$ 

• Smoothness: -  $f(\mathbf{x})$  is L-smooth on X if  $f(\mathbf{x})$  is differentiable

 $f(\mathbf{x}) \le f(\mathbf{y}) + \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y}) + \frac{L}{2} ||\mathbf{x} - \mathbf{y}||^2, \forall \mathbf{x}, \mathbf{y} \in X$ 

- 
$$f(\mathbf{x})$$
 is  $L$ -smooth **iff**  $\nabla f(\mathbf{x})$  is  $L$ -Lipschitz, i.e.,:

 $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \le L \|\mathbf{x} - \mathbf{y}\|, \forall \mathbf{x}, \mathbf{y}$ 

 $f\left(\mathbf{x} - \frac{1}{L}\nabla f(\mathbf{x})\right) - f(\mathbf{x}) \le -\frac{1}{2L}\|\nabla f(\mathbf{x})\|_{2}^{2}$ 

– If *f* is *L*-smooth then

and 
$$f(\mathbf{x}) - f(\mathbf{x}^*) \ge \frac{1}{2L} \|\nabla f(\mathbf{x})\|_2^2,$$
 (Proof see Hw6 Ex1)

- In all inequalities above, y is often set as  $\mathbf{x} - \frac{1}{T} \nabla f(\mathbf{x}).$ 

# • Strong convexity:

the PL inequality,

 $f(\mathbf{x}) \ge f(\mathbf{y}) + \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y}) + \frac{\mu}{2} ||\mathbf{x} - \mathbf{y}||^2, \forall \mathbf{x}, \mathbf{y} \in X$ - If f is  $\mu$ -strongly convex, then it also satisfies

• Smooth and Convex: If 
$$f(\mathbf{x})$$
 is convex and  $L$ -

 $\|\nabla f(\mathbf{x})\|_2^2 \ge 2\mu [f(\mathbf{x}) - f(\mathbf{x}^*)]$ 

 $f(\mathbf{y}) - f(\mathbf{x}) \le \nabla f(\mathbf{y})^{\top} (\mathbf{y} - \mathbf{x}) - \frac{1}{2I} ||\nabla f(\mathbf{y}) - \nabla f(\mathbf{x})||_2^2$ 

-  $f(\mathbf{x})$  is  $\mu$ -strongly convex on X if

$$[\nabla f(\mathbf{y}) - \nabla f(\mathbf{x})]^{\top} (\mathbf{y} - \mathbf{x}) \ge \frac{1}{L} ||\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})||$$

#### **Rate of Convergence** Consider the sequence $\{\delta_t\}_t \ge 0$ such that $\delta_0 \ge 0$ and

for some C > 0 and  $\alpha > 0$ .

 $\delta_t - \delta_{t+1} \ge C \cdot \delta_t^{\alpha}, \quad \forall t \ge 0$ 

For any 
$$\alpha > 1$$
, we have 
$$\delta_t = \mathcal{O}\left(\frac{1}{4^{1/(\alpha-1)}}\right)$$

For optimization problems, if we have

 $f(\mathbf{x}_t) - f(\mathbf{x}_{t+1}) \ge C \cdot (f(\mathbf{x}_t) - f^*)^{\alpha}, \quad \forall t \ge 0$ 

Then it implies that • If  $\alpha = 1$  and 0 < C < 1, then  $\{\mathbf{x}_t\}_t \ge 0$  achieves a

• If  $\alpha > 1$ , then  $\{\mathbf{x}_t\}_t > 0$  achieves a sublinear rate. • If  $\alpha < 1$ , then  $\{\mathbf{x}_t\}_t \ge 0$  achieves a superlinear rate.

 $g(\mathbf{x}) = f(\mathbf{x}) - f(\mathbf{x}^*) - \nabla f(\mathbf{x}^*)^{\top} (\mathbf{x} - \mathbf{x}^*)$ 

global minimizer. Construct the function

Then 
$$g(\mathbf{x})$$
 has a lot of properties:  
•  $g(\mathbf{x}) \ge 0$  and the equality is achieved when  $\mathbf{x} = \mathbf{x}^*$ .

Trick: Construction Related to Convex L-smooth

For a convex and *L*-smooth function f(x),  $\mathbf{x}^*$  is the

•  $g(\mathbf{x})$  is still *L*-smooth and convex.

•  $\nabla g(\mathbf{x}) = \nabla f(\mathbf{x}) - \nabla f(\mathbf{x}^*)$ . Thus,  $\nabla g(\mathbf{x}^*) = 0$  is the minimizer of  $g(\mathbf{x})$ 

# **Trick: Fundamental Theorem of Calculus** Goal: For a differentiable function $f: \mathbb{R}^d \to \mathbb{R}$ , ana-

lyze  $f(\mathbf{y}) - f(\mathbf{x})$  for all  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ . Trick: Consider function  $g(t) := f(\mathbf{x} + t(\mathbf{y} - \mathbf{x}))$ .  $\nabla g(t) = (\mathbf{y} - \mathbf{x})^{\top} \nabla f(\mathbf{x} + t(\mathbf{y} - \mathbf{x})).$ We can apply the fundamental theorem of calculus (theorem 2.4) twice for  $\Delta := g(1) - g(0)$ .

$$\Delta = f(\mathbf{y}) - f(\mathbf{x}) = \int_0^1 \nabla g(t) dt$$
 If  $f$  is twice-differentiable, then  $\nabla^2 g(t) = \int_0^1 \nabla g(t) dt$ 

 $(\mathbf{v} - \mathbf{x})^{\top} \nabla^2 f(\mathbf{x} + t(\mathbf{v} - \mathbf{x}))(\mathbf{v} - \mathbf{x}).$  $\Delta = f(\mathbf{y}) - f(\mathbf{x}) = \int_{0}^{1} \nabla g(t) dt$ 

$$\Delta = f(\mathbf{y}) - f(\mathbf{x}) = \int_0^t \nabla g(t) dt$$

$$= \int_0^1 \left( \int_0^t \nabla^2 g(z) dz + \nabla g(0) \right) dt$$
2. Convex Functions

## **Cauchy-Schwarz Inequality**

(1)  $|\langle \mathbf{u}, \mathbf{v} \rangle|^2 \le \langle \mathbf{u}, \mathbf{u} \rangle \cdot \langle \mathbf{v}, \mathbf{v} \rangle$ (2)  $\mathbf{x}^{\top} \mathbf{y} \leq \|\mathbf{x}\|_{2} \cdot \|\mathbf{y}\|_{2}$ 

(3)  $\mathbf{x}^{\top} \mathbf{y} \leq ||\mathbf{x}||_{\bullet} ||\mathbf{y}||_{*}$  in general.

 $(4) -1 \le \frac{\mathbf{u}^{\top} \mathbf{v}}{\|\mathbf{u}\| \|\mathbf{v}\|} \le 1$ 

(5) Triangle Ineq:  $||u + v|| \le ||u|| + ||v||$ 

(6)  $\|\mathbf{a} + \mathbf{b}\|_2^2 \le 2\|\mathbf{a}\|_2^2 + 2\|\mathbf{b}\|_2^2$ 

(7) Cosine:  $\cos \theta_{\mathbf{u}\mathbf{v}} = \frac{\langle \mathbf{u}, \mathbf{v} \rangle}{\|\mathbf{u}\| \|\mathbf{v}\|}$ 

(8) Var, Cov:  $Cov(X, Y)^2 \le Var(Y) Var(X)$ (9) Expectation:  $\mathbb{E}(XY)^2 \leq \mathbb{E}(X^2)\mathbb{E}(Y^2)$ 

# **Mean Value Theorem**

Let a < b,  $a, b \in \mathbb{R}$ , and  $h : [a, b] \to \mathbb{R}$  be a continuous func that is differentiable on (a, b). Then there exists  $c \in (a, b)$  s.t.

$$h'(c) = \frac{h(b) - h(a)}{b - a}$$

#### **Differentiable Functions** Optimization for Data Science Yilei Tu, Page 2 of 14

A set  $C \subseteq \mathbb{R}^d$  is convex if the line segment between any two points of C lies in C, i.e., if for any  $\mathbf{x}, \mathbf{y} \in C$ and any  $\lambda$  with  $0 \le \lambda \le 1$ , we have

$$\lambda \mathbf{x} + (1 - \lambda) \mathbf{y} \in C.$$

# Intersections of convex sets are convex.

#### **Convex Functions**

A function  $f : dom(f) \to \mathbb{R}$  is convex if (i) dom(f) is a convex set and (ii) for all  $\mathbf{x}, \mathbf{y} \in \text{dom}(f)$ , and  $\lambda$  with  $0 < \lambda < 1$ , we have

$$f(\lambda \mathbf{x} + (1 - \lambda)\mathbf{y}) \le \lambda f(\mathbf{x}) + (1 - \lambda)f(\mathbf{y})$$

• The graph of a function  $f: \mathbb{R}^d \to \mathbb{R}$  is defined as

$$\{(\mathbf{x}, f(\mathbf{x})) \mid \mathbf{x} \in \text{dom}(f)\}\$$

The **epigraph** of a function  $f: \mathbb{R}^d \to \mathbb{R}$  is defined

$$\operatorname{epi}(f) := \{ (\mathbf{x}, \alpha) \in \mathbb{R}^{d+1} \mid \mathbf{x} \in \operatorname{dom}(f), \alpha \ge f(\mathbf{x}) \},$$

• f is a convex function if and only if epi(f) is a convex set.

# Examples of convex functions

- Affine, Square, Exponential
- · Norm: Every norm is convex.

### **Convex Functions are Continuous**

# Let f be convex and suppose that $dom(f) \subseteq \mathbb{R}^d$ is open. Then f is continuous.

## Jensen's Inequality

Let f be convex,  $\mathbf{x}_1, \dots, \mathbf{x}_m \in \mathbf{dom}(f), \lambda_1, \dots, \lambda_m \in$  $\mathbb{R}_+$  such that  $\sum_{i=1}^m \lambda_i = 1$ . Then

$$f\left(\sum_{i=1}^{m} \lambda_i \mathbf{x}_i\right) \le \sum_{i=1}^{m} \lambda_i f\left(\mathbf{x}_i\right)$$

Expectation: If *X* is a random variable and  $\varphi$  is a convex function, then

$$\varphi(\mathbb{E}[X]) \le \mathbb{E}[\varphi(X)]$$

Let  $f: dom(f) \to \mathbb{R}^m$  where  $dom(f) \subseteq \mathbb{R}^d$  is open. f is called differentiable at  $\mathbf{x} \in \text{dom}(f)$  if there exists an  $(m \times d)$ -matrix **A** and an error function  $r: \mathbb{R}^d \to \mathbb{R}^m$  defined around  $\mathbf{0} \in \mathbb{R}^d$  such that for all y in some neighborhood of x,

$$f(\mathbf{y}) = f(\mathbf{x}) + \mathbf{A}(\mathbf{y} - \mathbf{x}) + r(\mathbf{y} - \mathbf{x})$$

where

$$\lim_{\mathbf{v}\to\mathbf{0}}\frac{\|r(\mathbf{v})\|}{\|\mathbf{v}\|}=\mathbf{0}.$$
 (Error  $r$  is sublinear)

- A is unique and called the differential or Jacobian matrix of f at  $\mathbf{x}$ .
- Graph of the affine function  $f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} \mathbf{x})$  is a tangent hyperplane to the graph of f at  $(\mathbf{x}, f(\mathbf{x}))$ . Lemma 2.15 First-order Characterization of Convexi-

f is convex if and only if dom(f) is convex and  $f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x})$  holds for all  $\mathbf{x}, \mathbf{y} \in \mathbf{dom}(f)$ .

f is convex if and only if dom(f) is convex, and for all  $\mathbf{x} \in \text{dom}(f)$ , we have  $\nabla^2 f(\mathbf{x}) \geq 0$ Lemma 2.16 Monotonicity of the Gradient Suppose that dom(f) is open and that f is differen-

Lemma 2.17 Second-order Characterization of Con-

tiable. Then f is convex iff dom(f) is convex and  $(\nabla f(\mathbf{y}) - \nabla f(\mathbf{x}))^{\top} (\mathbf{y} - \mathbf{x}) \ge 0$ 

holds for all 
$$\mathbf{x}, \mathbf{y} \in \text{dom}(f)$$
.

The inequality in monotonicity of the gradient is

## strict unless $\mathbf{x} = \mathbf{y}$ or $f(\lambda \mathbf{x} + (1 - \lambda)\mathbf{y}) = \lambda f(\mathbf{x}) + (1 - \lambda)\mathbf{y}$ $\lambda$ ) $f(\mathbf{y})$ for all $\lambda \in (0,1)$ .

# **Lemma 2.18 Operations that Preserve Convexity**

- (1) Let  $f_1, f_2, ..., f_m$  be convex functions,  $\lambda_1, \lambda_2, ..., \lambda_m \in \mathbb{R}_+$ . Then  $f := \max_{i=1}^m f_i$ as well as  $f := \sum_{i=1}^{m} \lambda_i f_i$  are convex on  $dom(f) := \bigcap_{i=1}^{m} dom(f_i)$ .
- (2) Let f be a **convex** function with  $dom(f) \subseteq$  $\mathbb{R}^d$ ,  $g: \mathbb{R}^m \to \mathbb{R}^d$ ,  $g(\mathbf{x}) = A\mathbf{x} + \mathbf{b}$ , for some matrix  $\mathbf{A} \in \mathbb{R}^{d \times m}$  and vector  $\mathbf{b} \in \mathbb{R}^d$ . Then the function  $f \circ g$  is convex on  $\text{dom}(f \circ g) :=$  $\{\mathbf{x} \in \mathbb{R}^m : g(\mathbf{x}) \in \text{dom}(f)\}.$

### **Local & Global Minima**

A local minimum of  $f: dom(f) \to \mathbb{R}$  is a point x such that there exists  $\varepsilon > 0$  with

$$f(\mathbf{x}) \le f(\mathbf{y}) \quad \forall \mathbf{y} \in \mathbf{dom}(f) \text{ satisfying } ||\mathbf{y} - \mathbf{x}|| < \varepsilon$$

Meaning: in some small neighborhood, **x** is the best point. **Lemma 2.20** Let  $\mathbf{x}^*$  be a local minimum of a convex function  $f: dom(f) \to \mathbb{R}$ . Then  $\mathbf{x}^*$  is a global minimum, meaning that  $f(\mathbf{x}^*) \leq f(\mathbf{y}) \quad \forall \mathbf{y} \in \text{dom}(f)$ .

#### **Lemma 2.22**

Suppose that  $f: dom(f) \to \mathbb{R}$  is differentiable over an open domain  $dom(f) \subseteq \mathbb{R}^d$ . Let  $\mathbf{x} \in dom(f)$ . If  $\mathbf{x}$  is a global minimum then  $\nabla f(\mathbf{x}) = \mathbf{0}$  (a critical point). **Lemma 2.21** 

For convex func, the converse of Lemma 2.22 is also true: If  $\nabla f(\mathbf{x}) = \mathbf{0}$ , then  $\mathbf{x}$  is a global minimum.

**Strictly Convex Functions** A function 
$$f : \text{dom}(f) \to \mathbb{R}$$
 is strictly convex if (i)

dom(f) is convex and (ii) for all  $\mathbf{x} \neq \mathbf{y} \in dom(f)$  and all  $\lambda \in (0,1)$ , we have

$$f(\lambda \mathbf{x} + (1 - \lambda)\mathbf{y}) < \lambda f(\mathbf{x}) + (1 - \lambda)f(\mathbf{y})$$

## **Lemma 2.25**

Strictly convex func has at most one global min. **Constrained Minimization** 

A point  $x \in X$  is a minimizer of f over X if  $f(\mathbf{x}) \le f(\mathbf{y}) \quad \forall \mathbf{y} \in X.$ 

Suppose that  $f: dom(f) \to \mathbb{R}$  is convex and differentiable over an open domain  $dom(f) \subseteq \mathbb{R}^d$ , and let  $X \subseteq \text{dom}(f)$  be a convex set. Point  $\mathbf{x}^* \in X$  is a

minimizer of 
$$f$$
 over  $X$  if and only if
$$\nabla f (\mathbf{x}^*)^\top (\mathbf{x} - \mathbf{x}^*) \ge 0 \quad \forall \mathbf{x} \in X$$

 $f: \mathbb{R}^d \to \mathbb{R}, \alpha \in \mathbb{R}$ . The set  $f^{\leq \alpha} := \{ \mathbf{x} \in \mathbb{R}^d : f(\mathbf{x}) \leq \alpha \}$ is the  $\alpha$ -sublevel set of f.

### Thm 2.29 (Weierstrass Theorem)

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be a convex function, and suppose there is a nonempty and bounded sublevel set  $f^{\leq \alpha}$ . Then f has a global minimum.

# **Optimization Problem in Standard Forms**

minimize 
$$f_0(\mathbf{x})$$
  
subject to  $f_i(\mathbf{x}) \le 0, \quad i = 1,...,m$   
 $h_i(\mathbf{x}) = 0, \quad i = 1,...,p$ 

Domain  $\mathcal{D} = \left\{ \bigcap_{i=0}^{m} \text{dom}(f_i) \right\} \cap \left\{ \bigcap_{i=1}^{p} \text{dom}(h_i) \right\}$ Convex program: All  $f_i$  are convex functions, and all  $h_i$  are affine functions with domain  $\mathbb{R}^d$ .

Lagrangian Given an optimization problem in standard form, its Lagrangian is the func  $L: \mathcal{D} \times \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}$  given

$$L(\mathbf{x}, \lambda, \nu) = f_0(\mathbf{x}) + \sum_{i=1}^{m} \lambda_i f_i(\mathbf{x}) + \sum_{i=1}^{p} \nu_i h_i(\mathbf{x})$$

The  $\lambda_i, v_i$  are called Lagrange multipliers. The Lagrange dual function is the function  $g: \mathbb{R}^m \times \mathbb{R}^p \to \mathbb{R}^p$  $\mathbb{R} \cup \{-\infty\}$  defined by

$$g(\lambda, \nu) = \inf_{\mathbf{x} \in \mathcal{D}} L(\mathbf{x}, \lambda, \nu).$$

## **Lemma 2.45 Weak Lagrange Duality**

Short Ver.: Lagrange dual function values are lower bounds on primal function values  $f_0(\mathbf{x})$ . Long Ver.: Let x be a feasible solution, meaning that  $f_i(\mathbf{x}) \leq 0$  for i = 1, ..., m and  $h_i(\mathbf{x}) = 0$  for i = 1, ..., p. Let g be the Lagrange dual function of and  $\lambda \in \mathbb{R}^m$ ,  $\nu \in \mathbb{R}^p$  such that  $\lambda \geq 0$ . Then

$$g(\lambda, \nu) \le f_0(\mathbf{x})$$

Choose  $\lambda \geq 0$  and  $\nu$  such that  $g(\lambda, \nu)$  is maximized! By weak duality, the supremum value of the Lagrange dual is a lower bound for the infimum value of the primal problem.

#### **Thm 2.47 Strong Lagrange Duality** Suppose that a convex program has a feasible soluti-

on  $\tilde{\mathbf{x}}$  that in addition satisfies  $f_i(\tilde{\mathbf{x}}) < 0, i = 1, ..., m$  (a Slater point). Then the infimum value of the primal equals the supremum value of its Lagrange dual. Moreover, if this value is finite, it is attained by a feasible solution of the dual. Convex programming with Slater point and finite value:  $\inf f_0(\mathbf{x}) = \max g(\lambda, \nu)$ .

# **Zero Duality Gap**

Let  $\tilde{\mathbf{x}}$  be feasible for the primal and  $(\tilde{\lambda}, \tilde{\nu})$  feasible for the Lagrange dual. The primal and dual solutions  $\tilde{\mathbf{x}}$  and  $(\tilde{\lambda}, \tilde{\mathbf{v}})$  are said to have zero duality gap if  $f_0(\tilde{\mathbf{x}}) = \varrho(\tilde{\lambda}, \tilde{\nu}).$ **Lemma 2.49 Complementary Slackness** 

# If $\tilde{\mathbf{x}}$ and $(\tilde{\lambda}, \tilde{\mathbf{v}})$ have zero duality gap, then

$$\tilde{\lambda}_i f_i(\tilde{\mathbf{x}}) = 0, \quad i = 1, \dots, m.$$

Lemma 2.50 Vanishing Lagrangian Gradient If  $\tilde{\mathbf{x}}$  and  $(\lambda, \tilde{\mathbf{v}})$  have zero duality gap, and if all  $f_i$  and  $h_i$  are differentiable, then

$$\nabla f_0(\tilde{\mathbf{x}}) + \sum_{i=1}^m \tilde{\lambda}_i \nabla f_i(\tilde{\mathbf{x}}) + \sum_{i=1}^p \tilde{v}_i \nabla h_i(\tilde{\mathbf{x}}) = \mathbf{0}$$

### **KKT Conditions**

- · primal and dual feasibilty
- · complementary slackness
- · vanishing Lagrangian gradient

$$f_i(\tilde{x}) \le 0, \quad i = 1, ..., m$$
  
 $h_i(\tilde{x}) = 0, \quad i = 1, ..., p$   
 $\tilde{\lambda}_i \ge 0, \quad i = 1, ..., m$   
 $\tilde{\lambda}_i f_i(\tilde{x}) = 0, \quad i = 1, ..., m$ 

$$\nabla f_0(\tilde{x}) + \sum_{i=1}^m \tilde{\lambda}_i \nabla f_i(\tilde{x}) + \sum_{i=1}^p \tilde{v}_i \nabla h_i(\tilde{x}) = 0$$

Suppose that all  $f_i$  and  $h_i$  are differentiable, all  $f_i$ 

 $(\mathbf{x}_t - \mathbf{x}_{t+1})/\gamma$ 

Vanilla Analysis

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optimal solutions.

are convex, all  $h_i$  are affine. Let  $\tilde{\mathbf{x}}$  and  $(\tilde{\lambda}, \tilde{\mathbf{v}})$  be such parameter  $2\|\mathbf{Q}\|_2$ . that the KKT conditions hold. Then  $\tilde{\mathbf{x}}$  and  $(\tilde{\lambda}, \tilde{\boldsymbol{\nu}})$  ha-Lemma 3.5 ve zero duality gap and hence are primal and dual Let  $f: \mathbb{R}^d \to \mathbb{R}$  be convex and differentiable. The following two statements are equivalent. 3. Gradient Descent (1) f is smooth with parameter L.

Lemma 3.3

• Gradient descent: Choose  $\mathbf{x}_0 \in \mathbb{R}^d \ \mathbf{x}_{t+1} := \mathbf{x}_t - \gamma \nabla f(\mathbf{x}_t)$  for times t = 0, 1, ..., and stepsize  $\gamma \geq 0$ . • Abbreviate:  $\mathbf{g}_t := \nabla f(\mathbf{x}_t)$  (gradient descent:  $\mathbf{g}_t =$ 

 $\mathbf{g}_{t}^{\top} \left( \mathbf{x}_{t} - \mathbf{x}^{\star} \right) = \frac{\gamma}{2} \|\mathbf{g}_{t}\|^{2} + \frac{1}{2\gamma} \left( \left\| \mathbf{x}_{t} - \mathbf{x}^{\star} \right\|^{2} - \left\| \mathbf{x}_{t+1} - \mathbf{x}^{\star} \right\|^{2} \right)$ 

Upper bound for the average error  $f(\mathbf{x}_t) - f(\mathbf{x}^*)$ over the first T iterations:  $\frac{1}{T} \sum_{t=0}^{T-1} \left( f\left(\mathbf{x}_{t}\right) - f\left(\mathbf{x}^{\star}\right) \right)$  $\leq \frac{1}{T} \left( \frac{\gamma}{2} \sum_{t=0}^{T-1} \|\mathbf{g}_t\|^2 + \frac{1}{2\gamma} \|\mathbf{x}_0 - \mathbf{x}^*\|^2 \right)$ 

Lipschitz Convex Func:  $\mathcal{O}(1/\varepsilon^2)$  Steps Assume that all gradients of f are bounded in norm. Equivalent to f being Lipschitz (Thm 2.9).

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be convex and differentiable with a global minimum x\*; furthermore, suppose that  $\|\mathbf{x}_0 - \mathbf{x}^*\| \le R$  and  $\|\nabla f(\mathbf{x})\| \le B$  for all  $\mathbf{x}$ . Choosing

the stepsize 
$$\gamma := \frac{R}{B\sqrt{T}}$$
 gradient descent yields 
$$\frac{1}{T} \sum_{t=0}^{T-1} \left( f\left(\mathbf{x}_{t}\right) - f\left(\mathbf{x}^{\star}\right) \right) \leq \frac{RB}{\sqrt{T}}$$

Average error  $\leq \frac{RB}{\sqrt{T}} \leq \varepsilon \Rightarrow T \geq \frac{R^2B^2}{\varepsilon^2}$ 

Let  $f: dom(f) \to \mathbb{R}$  be differentiable,  $X \subseteq dom(f)$ 

convex,  $L \in \mathbb{R}_+$  is called smooth (with parameter  $f(\mathbf{y}) \le f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{L}{2} ||\mathbf{x} - \mathbf{y}||^2, \quad \forall \mathbf{x}, \mathbf{y} \in X.$ 

 Does not require convexity. In general, quadratic functions are smooth.

• Affine functions are smooth with param 0.

• Iterative Algorithm: Choose  $\mathbf{x}_0 \in \mathbb{R}^d$ .  $\mathbf{x}_{t+1} :=$ (2)  $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \le L\|\mathbf{x} - \mathbf{y}\|$  for all  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$  $\mathbf{x}_t + \mathbf{v}_t$  for times t = 0, 1, ..., and steps  $\mathbf{v}_t \in \mathbb{R}^d$ . **Lemma 3.6 Operations that preserve smoothness** (1) Let  $f_1, f_2, ..., f_m$  be functions that are smooth with parameters  $L_1, L_2, ..., L_m$ , and let  $\lambda_1, \lambda_2, ..., \lambda_m \in \mathbb{R}_+$ . Then the function  $f := \sum_{i=1}^m \lambda_i f_i$  is smooth with parameter

Smoothness of  $f(\mathbf{x}) = \text{convexity of } \frac{L}{2} \mathbf{x}^{\top} \mathbf{x} - f(\mathbf{x})$ 

Let  $f(\mathbf{x}) = \mathbf{x}^{\top} \mathbf{O} \mathbf{x} + \mathbf{b}^{\top} \mathbf{x} + c$ , where **O** is a symmetric

 $(d \times d)$  matrix,  $\mathbf{b} \in \mathbb{R}^d$ ,  $c \in \mathbb{R}$ . Then f is smooth with

 $\sum_{i=1}^{m} \lambda_i L_i$ . (2) Let f be smooth with parameter L, and let  $g(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$ , for  $\mathbf{A} \in \mathbb{R}^{d \times m}$  and  $\mathbf{b} \in \mathbb{R}^d$ . Then the function  $f \circ g$  is smooth with parameter  $L||\mathbf{A}||_2^2$ . **Lemma 3.7 Sufficient Decrease** Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable and smooth with u) over X if

 $f(\mathbf{x}_{t+1}) \le f(\mathbf{x}_t) - \frac{1}{2I} \|\nabla f(\mathbf{x}_t)\|^2, \quad t \ge 0$ This doesn't require convexity. **Corollary of Sufficient Decrease Lemma** Let g be a L-smooth function and  $\mathbf{x}^*$  be a minimizer

parameter L. With stepsize  $\gamma := \frac{1}{L}$  gradient descent

of g. Then for any  $x \in dom(g)$ , we have  $g(\mathbf{x}) - g(\mathbf{x}^*) \ge \frac{1}{2L} \|\nabla g(\mathbf{x})\|_2^2$ 

Thm 3.8 Smooth Convex Func:  $\mathcal{O}(1/\varepsilon)$  Steps Let  $f: \mathbb{R}^d \to \mathbb{R}$  be convex and differentiable with a global minimum  $\mathbf{x}^*$ ; furthermore, suppose that f is smooth with parameter L. Choosing stepsize  $\gamma := \frac{1}{T}$  gradient descent yields  $f(\mathbf{x}_T) - f(\mathbf{x}^*) \le$  $\frac{L}{2T} \|\mathbf{x}_0 - \mathbf{x}^{\star}\|^2, \quad T > 0.$ 

Nesterov's Accelerated Gradient Descent (AGD): Let  $f: \mathbb{R}^d \to \mathbb{R}$  be convex, differentiable, and smooth with parameter L. Choose  $\mathbf{z}_0 = \mathbf{y}_0 = \mathbf{x}_0$  arbitrary. For  $t \geq 0$ , set

 $\mathbf{y}_{t+1} := \mathbf{x}_t - \frac{1}{L} \nabla f(\mathbf{x}_t)$ 

Let  $R^2 := \|\mathbf{x}_0 - \mathbf{x}^*\|^2$ , error  $\leq \frac{L}{2T} R^2 \leq \varepsilon \Rightarrow T \geq \frac{R^2 L}{2\varepsilon}$ 

 $\mathbf{z}_{t+1} := \mathbf{z}_t - \frac{t+1}{2L} \nabla f(\mathbf{x}_t)$  $\mathbf{x}_{t+1} := \frac{t+1}{t+3} \mathbf{y}_{t+1} + \frac{2}{t+3} \mathbf{z}_{t+1}$ 

(Proof see Hw6 Ex1)

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be convex and differentiable with a global minimum  $x^*$ ; furthermore, suppose that  $\varepsilon \Rightarrow T \geq \frac{L}{u} \ln \left( \frac{R^2 L}{2\varepsilon} \right)$ is smooth with parameter *L*. Accelerated gradient descent vields  $f(\mathbf{y}_T) - f(\mathbf{x}^*) \le \frac{2L \|\mathbf{z}_0 - \mathbf{x}^*\|^2}{T(T+1)}, \quad T > 0.$ 

**Potential Function of AGD** Define the **potential** as  $\Phi(t) := t(t+1) \left( f(\mathbf{y}_t) - f(\mathbf{x}^*) \right) + 2L \|\mathbf{z}_t - \mathbf{x}^*\|^2.$ 

**Thm 3.9 Error Bound of AGD** 

We can show that  $\Phi(t+1) \leq \Phi(t)$  for every t. Rewriting  $\Phi(T) \leq \Phi(0)$ , we can claim the error bound in (Proof see Handout03 Pages 29-30) **Strongly Convex Func** Let  $f: dom(f) \to \mathbb{R}$  be a convex and differentiable function,  $X \subseteq \text{dom}(f)$  convex and  $\mu \in \mathbb{R}_+, \mu > 0$ . Function *f* is called strongly convex (with parameter

 $f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{\mu}{2} ||\mathbf{x} - \mathbf{y}||^2, \quad \forall \mathbf{x}, \mathbf{y} \in X.$ **Lemma 3.11** Suppose that dom(f) is open and convex, and that

 $f: \operatorname{dom}(f) \to \mathbb{R}$  is differentiable. Let  $\mu \in \mathbb{R}_+$ . Then

the following two statements are equivalent. (i) f is

strongly convex with parameter  $\mu$ . (ii) g defined by  $g(\mathbf{x}) = f(\mathbf{x}) - \frac{\mu}{2} \mathbf{x}^{\mathsf{T}} \mathbf{x}$  is convex over dom(g) := dom(f). • *f* is *m*-strongly convex **iff**  $f''(\mathbf{x}) \ge m > 0$  for all  $\mathbf{x}$ .

**Lemma 3.12** 

If  $f: \mathbb{R}^d \to \mathbb{R}$  is strongly cvx with param  $\mu > 0$ , then f is strictly cvx and has a unique global min. Thm 3.14 Smooth and strongly convex func:  $\mathcal{O}(\log(1/\varepsilon))$  Steps

global minimum  $\mathbf{x}^*$ ; suppose that f is smooth with parameter L and strongly convex with parameter  $\mu > 0$ . Choosing  $\gamma := \frac{1}{L}$ , gradient descent with arbitrary  $\mathbf{x}_0$  satisfies the following two properties. (i) Squared distances to x\* are geometrically decrea-

 $\|\mathbf{x}_{t+1} - \mathbf{x}^{\star}\|^2 \le \left(1 - \frac{\mu}{L}\right) \|\mathbf{x}_t - \mathbf{x}^{\star}\|^2, \quad t \ge 0$ 

 $f(\mathbf{x}_T) - f(\mathbf{x}^*) \le \frac{L}{2} \left(1 - \frac{\mu}{L}\right)^T \|\mathbf{x}_0 - \mathbf{x}^*\|^2, \quad T > 0.$ 

 $\|\mathbf{x}_T - \mathbf{x}^{\star}\|^2 \le \left(1 - \frac{\mu}{I}\right)^T \|\mathbf{x}_0 - \mathbf{x}^{\star}\|^2$ (ii) The absolute error after T iterations is exponentially small in T:

ly require the function to be differentiable, and the gradient is replaced by the sub-gradient when the

A differentiable function f is said to have an L-Lipschitz continuous gradient if for some L > 0 $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \le L\|\mathbf{x} - \mathbf{y}\|, \forall \mathbf{x}, \mathbf{y}$ 

Let  $R^2 := \|\mathbf{x}_0 - \mathbf{x}^{\star}\|^2$ . Then error  $\leq \frac{L}{2} \left(1 - \frac{\mu}{L}\right)^T R^2 \leq 1$ 

Summary: Lipschitz Continuous Gradient (L-

Note: The definition **doesn't assume convexity** of f. (0)  $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \le L\|\mathbf{x} - \mathbf{y}\|, \forall \mathbf{x}, \mathbf{y}.$ 

(1)  $g(\mathbf{x}) = \frac{L}{2} \mathbf{x}^{\top} \mathbf{x} - f(\mathbf{x})$  is convex,  $\forall \mathbf{x}$ (2)  $f(\mathbf{y}) \le f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{L}{2} ||\mathbf{y} - \mathbf{x}||^2, \forall \mathbf{x}, \mathbf{y}.$ 

smoothness)

(3)  $(\nabla f(\mathbf{x}) - \nabla f(\mathbf{y}))^{\top} (\mathbf{x} - \mathbf{y}) \leq L ||\mathbf{x} - \mathbf{y}||^2, \forall \mathbf{x}, \mathbf{y}$  $(4) f(\alpha \mathbf{x} + (1 - \alpha)\mathbf{y}) \geq \alpha f(\mathbf{x}) + (1 - \alpha)f(\mathbf{y}) \frac{\alpha(1-\alpha)L}{2} \|\mathbf{x} - \mathbf{y}\|^2, \forall \mathbf{x}, \mathbf{y} \text{ and } \alpha \in [0,1]$ 

 $\nabla f(\mathbf{x})||^2, \forall \mathbf{x}, \mathbf{y}.$ 

(5)  $f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{1}{2L} \|\nabla f(\mathbf{y}) - \mathbf{y}\|$ 

 $\geq$ 

 $\frac{1}{T} ||\nabla f(\mathbf{x})|| -$ 

(6)  $(\nabla f(\mathbf{x}) - \nabla f(\mathbf{y}))^{\top} (\mathbf{x} - \mathbf{y})$  $\nabla f(\mathbf{y})||^2, \forall \mathbf{x}, \mathbf{v}$ (7)  $f(\alpha \mathbf{x} + (1 - \alpha)\mathbf{y}) \leq \alpha f(\mathbf{x}) + (1 - \alpha)f(\mathbf{y}) \frac{\alpha(1-\alpha)}{2^T} \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|^2, \forall \mathbf{x}, \mathbf{y} \text{ and } \alpha \in [0,1]$ 

Note: We assume that the domain for *f* and *g* are both  $\mathbb{R}^n$ , and hence convex set. Let  $f: \mathbb{R}^d \to \mathbb{R}$  be convex and differentiable with a

For a function f with a Lipschitz continuous gradient over  $\mathbb{R}^n$ , the following implications hold:

 $[5] \equiv [7] \rightarrow [6] \rightarrow [0] \rightarrow [1] \equiv [2] \equiv [3] \equiv [4]$ 

If we further assume that f is convex, then we have all the conditions [0] - [7] are equivalent.

# **Summary: Strong Convexity**

function is non-smooth.

A differentiable function f is strongly convex if  $f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{\mu}{2} ||\mathbf{y} - \mathbf{x}||^2$  for some  $\mu > 0$ and all x, y Note: Strong convexity doesn't necessari-

Optimization for Data Science Yilei Tu, Page 4 of 14 Equivalent Conditions of Strong Convexity

# The following conditions are all equivalent to the

condition that a differentiable function f is stronglyconvex with constant  $\mu > 0$ . (i)  $f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{\mu}{2} ||\mathbf{y} - \mathbf{x}||^2, \forall \mathbf{x}, \mathbf{y}.$ 

- (ii)  $g(\mathbf{x}) = f(\mathbf{x}) \frac{\mu}{2} ||\mathbf{x}||^2$  is convex,  $\forall x$ .
- (iii)  $(\nabla f(\mathbf{x}) \nabla f(\mathbf{y}))^{\top} (\mathbf{x} \mathbf{y}) \ge \mu ||\mathbf{x} \mathbf{y}||^2, \forall \mathbf{x}, \mathbf{y}.$ (iv)  $f(\alpha \mathbf{x} + (1 - \alpha)\mathbf{y}) \leq \alpha f(\mathbf{x}) + (1 - \alpha)f(\mathbf{y}) -$
- $\frac{\alpha(1-\alpha)\mu}{2} \|\mathbf{x} \mathbf{y}\|^2, \alpha \in [0,1].$

For a continuously differentiable function f, the following conditions are all implied by strong convexity (SC) condition.

- (a)  $\frac{1}{2} \|\nabla f(\mathbf{x})\|^2 \ge \mu(f(\mathbf{x}) f^*), \forall \mathbf{x}.$
- (b)  $\|\nabla f(\mathbf{x}) \nabla f(\mathbf{y})\| \ge \mu \|\mathbf{x} \mathbf{y}\| \forall \mathbf{x}, \mathbf{y}.$
- (c)  $f(\mathbf{y}) \leq f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} \mathbf{x}) + \frac{1}{2u} ||\nabla f(\mathbf{y})||$
- $\nabla f(\mathbf{x})||^2, \forall \mathbf{x}, \mathbf{v}.$
- (d)  $(\nabla f(\mathbf{x}) \nabla f(\mathbf{y}))^{\top} (\mathbf{x} \mathbf{y}) \leq$  $\nabla f(\mathbf{y})||^2, \forall \mathbf{x}, \mathbf{y}$
- **Additivity of Strongly Convex Functions**

#### Assume that real functions f is a-strongly convex and g is b-strongly convex. Then the sum f + g is

- also strongly convex, with parameter a + b. (Proof see GA2 Solution6) Let h = f + g where f is strongly convex with pa-
- ram  $\mu$  and g is convex, then h is strongly convex with param  $\mu$ . 4a. Projected Gradient Descent

# **Constrained Optimization Problem**

minimize  $f(\mathbf{x})$ subject to  $\mathbf{x} \in X, X \subseteq \mathbb{R}^d$  (closed convex set)

# **Projected Gradient Descent**

Choose  $\mathbf{x}_0 \in \mathbb{R}^d$ .

see Hw4 Ex1)

$$\mathbf{y}_{t+1} := \mathbf{x}_t - \gamma \nabla f(\mathbf{x}_t)$$
  
$$\mathbf{x}_{t+1} := \Pi_X(\mathbf{y}_{t+1}) := \underset{\mathbf{x} \in X}{\operatorname{argmin}} \|\mathbf{x} - \mathbf{y}_{t+1}\|^2$$

for times t = 0, 1, ..., and stepsize  $\gamma \ge 0$ .

- When  $\nabla f(\mathbf{x}_t) \neq \mathbf{0}$  but  $\mathbf{x}_{t+1} = \mathbf{x}_t$  (convex f and X), we have reached an optimal solution: the gradient is orthogonal to a hyperplane through  $\mathbf{x}_t$  that has all feasible solutions on one side.
- $f(\mathbf{x}_{t+1}) \leq f(\mathbf{x}_t)$  (Proof see Hw4 Ex1)  $\|\mathbf{y}_{t+1} - \mathbf{x}_{t+1}\| \le \|\mathbf{y}_{t+1} - \mathbf{x}_t\| = \gamma \|\nabla f(\mathbf{x}_t)\|$  (Proof

**Optimality Condition for Projected Gradient Descent** Using projected gradient descent,  $\mathbf{x}^*$  is an optimal solution to the constrained optimization problem iff  $\mathbf{x}^* = \prod_{\gamma} \left( \mathbf{x}^* - \gamma \nabla f \left( \mathbf{x}^* \right) \right)$ (Proof see ODS Exam FS20 Assignment 2) **Fact 4a.1 Properties of Projection** 

Let  $X \subseteq \mathbb{R}^d$  closed and convex,  $\mathbf{x} \in X, \mathbf{y} \in \mathbb{R}^d$ . Then (i)  $(\mathbf{x} - \Pi_X(\mathbf{y}))^{\top} (\mathbf{y} - \Pi_X(\mathbf{y})) \leq 0$ .

- (ii)  $\|\mathbf{x} \Pi_X(\mathbf{y})\|^2 + \|\mathbf{y} \Pi_X(\mathbf{y})\|^2 \le \|\mathbf{x} \mathbf{y}\|^2$ .

**Num of Steps for PGD** The same number of steps as GD over  $\mathbb{R}^d$ !

- Lipschitz convex functions over  $X : \mathcal{O}(1/\varepsilon^2)$  steps
- Smooth convex functions over  $X : \mathcal{O}(1/\varepsilon)$  steps • Smooth and strongly convex functions over *X* :
- $\mathcal{O}(\log(1/\varepsilon))$  steps **Lemma 4a.3 Projected Sufficient Decrease**

Let  $f: dom(f) \to \mathbb{R}$  be differentiable and smooth with parameter L over a closed and convex set

 $X \subseteq \text{dom}(f)$ . Choosing stepsize  $\gamma := \frac{1}{f}$ , projected gradient descent with arbitrary  $\mathbf{x}_0 \in X$  satisfies, for

Thm 4a.4 Smooth Convex Func over 
$$X : \mathcal{O}(1/\varepsilon)$$
 Steps Let  $f : \text{dom}(f) \to \mathbb{R}$  be convex and differentiable.

 $f(\mathbf{x}_{t+1}) \le f(\mathbf{x}_t) - \frac{1}{2L} \|\nabla f(\mathbf{x}_t)\|^2 + \frac{L}{2L} \|\mathbf{y}_{t+1} - \mathbf{x}_{t+1}\|^2$ 

Let  $X \subseteq \text{dom}(f)$  be a closed convex set, and assume that there is a minimizer  $\mathbf{x}^*$  of f over X; furthermore, suppose that f is smooth over X with parameter L. Choosing stepsize  $\gamma := \frac{1}{L}$ , projected gradient descent yields

$$f(\mathbf{x}_{t+1}) \le f(\mathbf{x}_t)$$

 $\frac{1}{u}||\nabla f(\mathbf{x})||$ 

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \le \frac{L}{2T} \|\mathbf{x}_0 - \mathbf{x}^*\|^2, \quad T > 0.$$

Exactly the same bound as in the unconstrained

#### 4b. Coordinate Descent PL Inequality

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be a differentiable function with a

 $\frac{1}{2} \|\nabla f(\mathbf{x})\|^2 \ge \mu (f(\mathbf{x}) - f(\mathbf{x}^*)), \quad \forall \mathbf{x} \in \mathbb{R}^d$ 

global minimum 
$$\mathbf{x}^*$$
. We say that  $f$  satisfies the PL inequality if the following holds for some  $\mu > 0$ :

Direct consequence:  $\nabla f(\mathbf{x}) = \mathbf{0} \Rightarrow \mathbf{x}$  is a global min. Lemma 4b.2 Strong convexity ⇒ PL inequality

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable and strongly convex with parameter  $\mu > 0$  (in particular, a global minimum  $x^*$  exists by Lemma 3.12). Then f satisfies the PL inequality for the same  $\mu$ .

Thm 4b.3 GD on Smooth Func with PL Ineq Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable with a global min

 $\mathbf{x}^{\star}$ . Suppose that f is smooth with param L and satisfies the PL ineq with param  $\mu > 0$ . Choosing stepsize  $\gamma = 1/L$ , GD with arbitrary  $\mathbf{x}_0$  satisfies

$$f(\mathbf{x}_T) - f(\mathbf{x}^*) \le \left(1 - \frac{\mu}{L}\right)^T (f\mathbf{x}_0) - f(\mathbf{x}^*), \quad T > 0$$

Coordinate-wise Smoothness

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable, and  $\mathcal{L} =$ 

 $(L_1, L_2, \dots, L_d) \in \mathbb{R}^d_+$ . Func f is called coordinatewise smooth (with param  $\mathcal{L}$  ) if for every coordinate i = 1, 2, ..., d,

$$f(\mathbf{x} + \lambda \mathbf{e}_i) \le f(\mathbf{x}) + \lambda \nabla_i f(\mathbf{x}) + \frac{L_i}{2} \lambda^2 \quad \forall \mathbf{x} \in \mathbb{R}^d, \lambda \in \mathbb{R},$$

• If  $L_i = L$  for all i, f is said to be coordinate-wise

- smooth with param *L*. • If f is smooth with param L, then f is coordinatewise smooth with param L.
- **Coordinate Descent Algo** In Iteration *t*:
  - (i) Choose some  $i \in [d]$
- (ii)  $\mathbf{x}_{t+1} := \mathbf{x}_t \gamma_i \nabla_i f(\mathbf{x}_t) \mathbf{e}_i$ •  $\nabla_i f(\mathbf{x}_t)$  is the *i*-th entry of the gradient (*i*-th par-
- tial derivate). • **e**<sub>i</sub> is the *i*-th unit vector, so only the *i*-th coordina-
- te of  $\mathbf{x}_t$  is updated.
- $\gamma_i$  is the stepsize for coordinate *i*. **Lemma 4b.5 Coordinate-wise Sufficient Decrease**

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable and coordinatewise smooth with parameter  $\mathcal{L} = (L_1, L_2, ..., L_d)$ . With active coordinate i in iteration t and stepsize  $\gamma_i = \frac{1}{L}$ , coordinate descent satisfies

$$f(\mathbf{x}_{t+1}) \le f(\mathbf{x}_t) - \frac{1}{2L_i} \|\nabla_i f(\mathbf{x}_t)\|^2$$

**Randomized Coordinate Descent** 

- (i) sample  $i \in [d]$  uniformly at random
- (ii)  $\mathbf{x}_{t+1} := \mathbf{x}_t \gamma_i \nabla_i f(\mathbf{x}_t) \mathbf{e}_i$

**Thm 4b.6 Randomized Coordinate Descent: Smooth** Func, PL inequality Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable with a global mini-

mum  $\mathbf{x}^{\star}$ . Suppose that f is coordinate-wise smooth with parameter L and satisfies the PL inequality with parameter  $\mu > 0$ . Choosing stepsize  $\gamma_i = 1/L$ for all coordinates, randomized coordinate descent with arbitrary  $\mathbf{x}_0$  satisfies

$$\mathbb{E}\left[f\left(\mathbf{x}_{T}\right) - f\left(\mathbf{x}^{\star}\right)\right] \leq \left(1 - \frac{\mu}{dL}\right)^{T} \left(f\left(\mathbf{x}_{0}\right) - f\left(\mathbf{x}^{\star}\right)\right)$$

**Importance Sampling** 

Improves over uniform sampling when coordinatewise smoothness parameters  $L_i$  differ.

- (i) sample  $i \in [d]$  with probability  $\frac{L_i}{\sum_{i=d}^{d} L_i}$ (ii)  $\mathbf{x}_{t+1} := \mathbf{x}_t - \frac{1}{L} \nabla_i f(\mathbf{x}_t) \mathbf{e}_i$

Thm 4b.7 Convergence of Importance Sampling

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable with a global min  $\mathbf{x}^{\star}$ , coordinate-wise smooth with param  $\mathcal{L} =$  $(L_1, L_2, ..., L_d)$ , and satisfying the PL ineq with pa-

$$\mathbb{E}\left[f\left(\mathbf{x}_{T}\right) - f\left(\mathbf{x}^{\star}\right)\right] \leq \left(1 - \frac{\mu}{dT}\right)^{T} \left(f\left(\mathbf{x}_{0}\right) - f\left(\mathbf{x}^{\star}\right)\right)$$

ram  $\mu > 0$ . Let  $\overline{L} = \frac{1}{d} \sum_{i=1}^{d} L_i$ . Then coordinate de-

scent with importance sampling and arbitrary  $\mathbf{x}_0$ 

Corollary 4b.8

Same number of iterations as randomized coordinate descent. Strong convexity wrt  $\ell_1$ -norm

• Measure strong convexity wrt  $\ell_1$ -norm instead of

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{\mu_1}{2} ||\mathbf{y} - \mathbf{x}||_1^2, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^d$$

• Then f is also strongly convex with  $\mu = \mu_1$  in the usual sense. Proof:  $\|\mathbf{y} - \mathbf{x}\|_1 \ge \|\mathbf{y} - \mathbf{x}\|_2$ 

• If f is strongly convex with  $\mu$  in the usual sen-

se, then f is strongly convex with  $\mu_1 = \mu/d$  w.r.t.  $\ell_1$ -norm.

Proof:  $\|\mathbf{y} - \mathbf{x}\| \ge \|\mathbf{y} - \mathbf{x}\|_1 / \sqrt{d}$ 

- $\mu \ge \mu_1 \ge \mu/d$
- If  $\mu_1 > \mu/d$ , we can speed up steepest coordinate descent.

Lemma 4b.9 Strong convexity w.r.t.  $\ell_1$ -norm  $\Rightarrow$  PL inequality w.r.t.  $\ell_{\infty}$ -norm

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable and strongly convex with parameter  $\mu_1 > 0$  w.r.t.  $\ell_1$ -norm. (In particular, f is  $\mu_1$ -strongly convex w.r.t. Euclidean norm, so a global minimum  $x^*$  exists by Lemma 3.12). Then f satisfies the PL inequality w.r.t.  $\ell_{\infty}$ -norm with the

 $\frac{1}{2} \|\nabla f(\mathbf{x})\|_{\infty}^2 \ge \mu_1 \left( f(\mathbf{x}) - f(\mathbf{x}^*) \right), \quad \forall \mathbf{x} \in \mathbb{R}^d$ 

Optimization for Data Science Yilei Tu, Page 5 of 14 Thm 4b.10 Steeper (than steepest) coordinate de-

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable with a global minimum  $\mathbf{x}^{\star}$ . Suppose that f is coordinate-wise smooth with parameter *L* and satisfies the PL inequality w.r.t.

 $\ell_{\infty}$ -norm with parameter  $\mu_1 > 0$ . Choosing stepsize  $\gamma_i = 1/L$ , steepest coordinate descent with arbitrary

• Normal steepest coordinate descent: 
$$\left(1 - \frac{\mu_1}{L}\right)^T \left(f(\mathbf{x}_0) - f(\mathbf{x}^*)\right)$$
,  $T > 0$ 

- Worst case:  $\mu_1 = \mu/d$ , no speedup. • Best case:  $\mu_1 = \mu$ , speedup by a factor of d.
- **Greedy Coordinate Descent** Make the step that maximizes the progress in the

This requires to perform a line search.

- chosen coordinate! (i) choose  $i \in [d]$
- (ii)  $\mathbf{x}_{t+1} := \operatorname{argmin} f(\mathbf{x}_t + \lambda \mathbf{e}_i)$

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be of the form

$$f(\mathbf{x}) := g(\mathbf{x}) + h(\mathbf{x})$$
 with  $h(\mathbf{x}) = \sum_{i} h_i(x_i)$ ,  $\mathbf{x} \in \mathbb{R}^d$ 

with g convex and differentiable, and the  $h_i$  convex.

Norm |

Let  $\mathbf{x} \in \mathbb{R}^d$  be a point such that greedy coordinate descent cannot make progress in any coordinate. Then **x** is a global minimum of f. A function h as in the theorem is called separable. Popular examples: regularizers  $h(\mathbf{x}) = \|\mathbf{x}\|_1$  and

Smooth

 $h(\mathbf{x}) = ||\mathbf{x}||^2.$ Summary

Algo Rand

IS Steepest

Steeper

gradient descent. 5. Subgradient Methods

(3) Squared loss:  $f(s) = (s-1)^2$ 

**Bounded Subgradients** 

Thm 4b.7 Lemma 5.7 Subgradient optimality condition Coro 4b.8 Suppose that  $f : \text{dom}(f) \to \mathbb{R}$  and  $\mathbf{x} \in \text{dom}(f)$ . If  $0 \in \partial f(\mathbf{x})$ , then  $\mathbf{x}$  is a global min. Thm 4b.10 Calculus of Subgradient and Subdifferential

In the worst case, nothing is gained over gradient
• Conic combination: Let  $h(\mathbf{x}) = \beta_1 f_1(\mathbf{x}) + \beta_2 f_2(\mathbf{x})$ descent, and Steepest may even lose. In the best case, Importance sampling and Steeper

(1) 0-1 Loss:  $f(s) = \begin{cases} 1, & s < 0 \\ 0, & s \ge 0 \end{cases}$ (2) Hinge losss:  $f(s) = \max(0, 1-s)$ 

$$f(s) = (s-1)^2$$

(4) Exponential loss:  $f(s) = e^{-s}$ 

- (5) Logistic loss:  $f(s) = \log(1 + e^{-s})$

- (1) non-convex, (2)-(5) convex. (1)(2)(4) non-smooth, (3)(5) smooth. Subgradients

 $\mathbf{g} \in \mathbb{R}^d$  is a subgradient (not always unique) of f at

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{g}^{\top}(\mathbf{y} - \mathbf{x})$$
 for all  $\mathbf{y} \in \text{dom}(f)$ 

$$f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{g}^{\top}(\mathbf{y} - \mathbf{x})$$
 for all  $\mathbf{y} \in \text{dom}(f)$   $\partial f(\mathbf{x}) \subseteq \mathbb{R}^d$  is the subdifferential, the set of subgradients of  $f$  at  $\mathbf{x}$ .

**Lemma 5.2 Subgradients of Differentiable Func** If f is differentiable at  $\mathbf{x} \in \mathbf{dom}(f)$ , then  $\partial f(\mathbf{x}) \subseteq$  $\{\nabla f(\mathbf{x})\}.$ 

i.e., either exactly one subgradient  $\nabla f(\mathbf{x})$ , or no sub-

gradient at all. **Lemma 5.3 Subgradient Characterization of Conve-**

(i) If f is convex, then  $\partial f(\mathbf{x}) \neq \emptyset$  for all  $\mathbf{x}$  in the

- (relative) interior of dom(f). (ii) If dom(f) is convex and  $\partial f(\mathbf{x}) \neq \emptyset$  for all
- $\mathbf{x} \in \text{dom}(f)$ , then f is convex. i.e., convex = subgradients everywhere.

Thm 5.4 Hyperplane Separation Theorem Two nonempty convex sets can be separated by a hyperplane if their (relative) interiors do not intersect.

Thm 5.5 Differentiability of convex functions A **convex** function *f* is differentiable **almost every**where on dom(f). **Lemma 5.6 Convex and Lipschitz continuity** ← →

Let  $f : \text{dom}(f) \to \mathbb{R}$  be convex, dom(f) open,  $B \in \mathbb{R}_+$ . Then the following two statements are equivalent: (i)  $\|\mathbf{g}\|_2 \leq B$  for all  $\mathbf{x} \in \text{dom}(f)$  and all  $\mathbf{g} \in \partial f(\mathbf{x})$ .

- (ii)  $|f(\mathbf{x}) f(\mathbf{y})| \le B||\mathbf{x} \mathbf{y}||_2$  for all  $\mathbf{x}, \mathbf{y} \in \text{dom}(f)$ .
- More generally, let  $f: S \to \mathbb{R}$  be a convex function. Then, f is L- Lipschitz over S with respect to a norm  $\|\cdot\|$  iff for all  $\mathbf{w} \in S$  and  $\mathbf{z} \in \partial f(\mathbf{w})$  we have that
- Thm  $4b.6 \|\mathbf{z}\|_{\star} \leq L$ , where  $\|\cdot\|_{\star}$  is the dual norm.

with  $\beta_1$ ,  $\beta_2 \ge 0$ , then  $\partial h(\mathbf{x}) = \beta_1 \partial f_1(\mathbf{x}) + \beta_2 \partial f_2(\mathbf{x})$ (than Steepest) may be up to d times faster than • Affine transformation: Let h(x) = f(Ax + b), then

> • Pointwise maximum: Let  $h(\mathbf{x}) = \max_{i=1,...,m} f_i(\mathbf{x})$ , then  $\partial h(x) = \text{conv} \{ \partial f_i(\mathbf{x}) : i \text{ such that } f_i(\mathbf{x}) = h(\mathbf{x}) \}$

> Negative subgradient may not be a descent directi-

 $\partial h(\mathbf{x}) = A^{\top} \partial f(A\mathbf{x} + b)$ 

(convex hull)

minimize  $f(\mathbf{x})$ subject to  $\mathbf{x} \in X$ Assume that •  $f(\mathbf{x})$  is convex and B-Lipschitz continuous on X:

 $|f(\mathbf{x}) - f(\mathbf{y})| \le B||\mathbf{x} - \mathbf{y}||_2$ ,  $\forall \mathbf{x}, \mathbf{y} \in X$ . This implies that  $\|\mathbf{g}\|_2 \leq B$  for any  $\mathbf{g} \in \partial f(x)$ .

• X is convex and compact:  $R := \max_{\mathbf{x}, \mathbf{y} \in X} ||\mathbf{x} - \mathbf{y}||_2 < +\infty$ .

Denote  $X^*$  as the optimal set such that  $X^* \neq \emptyset$ . Denote  $f^*$  as the optimal value such that  $f^* < \infty$ .

**Subgradient Descent** Choose  $\mathbf{x}_1 \in \mathbb{R}^d$ .  $\mathbf{x}_{t+1} := \Pi_X \left( \mathbf{x}_t - \gamma_t \mathbf{g}_t \right)$ 

**Convex Nonsmooth Problem Setting** 

 $= \underset{\mathbf{x} \in Y}{\operatorname{argmin}} \left\{ \frac{1}{2} \|\mathbf{x} - \mathbf{x}_t\|_2^2 + \langle \gamma_t \mathbf{g}_t, \mathbf{x} \rangle \right\}, \mathbf{g}_t \in \partial f(\mathbf{x}_t)$ •  $\mathbf{g}_t$  is a subgradient of f at  $\mathbf{x}_t$ .

- $\gamma_t > 0$  is a proper (time-varying) stepsize. •  $\Pi_X(\mathbf{y}) := \operatorname{argmin}_{\mathbf{x} \in X} \|\mathbf{x} - \mathbf{y}\|_2^2$  is the **projection**. • When *f* is differentiable and  $X = \mathbb{R}^d$ , this reduces
- to Gradient Descent. • When f is differentiable and  $X \subset \mathbb{R}^d$ , this reduces to Projected Gradient Descent.
- When f is non-differentiable, we see that it is not always a descent method.
- **Choices of Stepsize** • Constant stepsize:  $\gamma_t = \gamma$
- Scaled stepsize:  $\gamma_t = \frac{\gamma}{\|q_t\|_2}$ • Non-summable but diminishing stepsize:  $\gamma_t \rightarrow 0$
- and  $\sum_{t=1}^{\infty} \gamma_t = +\infty$ , e.g.:  $\gamma = \mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$ • Square summable stepsize:  $\sum_{t=1}^{\infty} \gamma_t^2 < +\infty$  and  $\sum_{t=1}^{\infty} \gamma_t = +\infty$ , e.g.:  $\gamma = \mathcal{O}\left(\frac{1}{t}\right)$
- Polyak's stepsize:  $\gamma_t = \frac{f(\mathbf{x}_t) f^*}{\|\mathbf{g}_t\|_2^2}$ , where  $f^*$  is the optimal value.

**Lemma 5.8 Basic Descent Lemma** If f is convex (and B-Lipschitz), then for any optimal solution  $\mathbf{x}^* \in X^*$ .

 $\|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \le \|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - 2\gamma_t (f(\mathbf{x}_t) - f^*) + \gamma_t^2 \|\mathbf{g}_t\|_2^2$  $\Rightarrow \|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \le \|\mathbf{x}_t - \mathbf{x}^*\|_2^2 + \gamma_t^2 \|\mathbf{g}_t\|_2^2$  $\Rightarrow \|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \le \|\mathbf{x}_t - \mathbf{x}^*\|_2^2 + \gamma_t^2 B^2$ 

 $\Rightarrow \|\mathbf{x}_{T} - \mathbf{x}^{*}\|_{2}^{2} \leq \|\mathbf{x}_{t_{k}} - \mathbf{x}^{*}\|_{2}^{2} + B^{2} \sum_{t=1}^{I-1} \gamma_{t}^{2}$ 

 $\min_{1 \leq t \leq T} f\left(\mathbf{x}_{t}\right) - f^{*} \leq \frac{\|\mathbf{x}_{1} - \mathbf{x}^{*}\|_{2}^{2} + \sum_{t=1}^{T} \gamma_{t}^{2} \|\mathbf{g}_{t}\|_{2}^{2}}{2 \sum_{t=1}^{T} \gamma_{t}^{2}}$ 

Thm 5.9 Main Theorem on Convergence

If f is convex, then the subgradient method satisfies:

**Asymptotic Convergence under Different Stepsizes** Recall  $\|\mathbf{x}_t - \mathbf{x}^*\| \le R^2$  and  $\|\mathbf{g}_t\|_2^2 \le B^2$ 

• Constant  $\gamma_t \equiv \gamma$ :  $\liminf_{t \to \infty} f(\mathbf{x}_t) \le f^* + B^2 \gamma / 2$ • Scaled  $\gamma_t = \frac{\gamma}{\|g_t\|_2}$ :  $\liminf_{t \to \infty} f(\mathbf{x}_t) \le f^* + B\gamma/2$ • Square-summable  $\sum_{t=1}^{\infty} \gamma_t^2 < +\infty$  and  $\sum_{t=1}^{\infty} \gamma_t =$ 

 $+\infty$ :  $\liminf_{t\to\infty} f(\mathbf{x}_t) = f'$ • Diminishing  $\gamma_t \rightarrow 0$  and  $\sum_{t=1}^{\infty} \gamma_t = +\infty$ :  $\liminf_{t\to\infty} f(\mathbf{x}_t) = f^*$ 

**Subgradient Descent Convergence under Polyak's** Minimizing the surrogate func in Lemma 5.8 yields the optimal stepsize (**Polyak**):  $\gamma_t = \frac{f(\mathbf{x}_t) - f^*}{\mathbf{y}_t - \mathbf{y}_t^2}$ 

This guarantees strict error reduction (\*):

 $\|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \le \|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - \frac{(f(\mathbf{x}_t) - f^*)^2}{\|g(\mathbf{x}_t)\|_2^2}$ 

It follows that  $f(\mathbf{x}_t) \to f^*$  and  $\{\mathbf{x}_t\} \to \mathbf{x}^*$ . Polyak's Stepsize is useful when the optimal value  $f^*$  is known, but minimizer  $\mathbf{x}^*$  is unknown.

In practice, the opt value is often not available. One can replace  $f^*$  by an online estimate, e.g.,  $\hat{f}_t := \min_{0 \le \tau \le t} f(\mathbf{x}_{\tau}) - \delta$ 

> • Assume f is convex and B-Lipscitz, then (\*) im- $\min_{1 \le t \le T} f(\mathbf{x}_t) - f(\mathbf{x}^*) \le \frac{B \|\mathbf{x}_1 - \mathbf{x}^*\|_2}{\sqrt{T}}$

(Proof see Hw5 Ex4.1) • Assume f is  $\mu$  strongly convex and B-Lipscitz.

In the case where f is non-differentiable, the definition of strong convexity we saw in lecture

no longer applies. However, we can still define strong convexity in this setting as follows: For  $\mu > 0$ , A function f is said to be  $\mu$ -strongly convex if the function  $f_{\mu}(x) := f(\mathbf{x}) - \frac{\mu}{2} ||\mathbf{x}||^2$  is convex. Let f be  $\mu$ -strongly convex, then for all  $\mathbf{x}$ ,  $\mathbf{y}$  in the domain and for all  $\mathbf{g} \in \partial f(\mathbf{x})$  we have  $f(\mathbf{y}) \ge f(\mathbf{x}) + \mathbf{g}^{\top}(\mathbf{y} - \mathbf{x}) + \frac{\mu}{2} ||\mathbf{x} - \mathbf{y}||^2.$ 

Then (\*) implies

 $\min_{1 < t < T} f(\mathbf{x}_t) - f(\mathbf{x}^*) \le \frac{4B^2}{\mu T}$ 

(Proof see Hw5 Ex4.2)

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If *f* is convex and *B*-Lipschitz continuous, and *X* is convex compact with diameter R. Let  $\gamma_t \equiv \frac{R}{R\sqrt{T}}$  or

Corollary 5.10 Convergence Rate for Convex Lip-

 $\gamma_t = \frac{R}{R\sqrt{t}}$ , then

$$\min_{1 \le t \le T} f(\mathbf{x}_t) - f^* \le \mathcal{O}\left(\frac{BR}{\sqrt{T}}\right)$$

- Subgradient method converges sublinearly.
- For an accuracy  $\epsilon > 0$ , need  $\mathcal{O}\left(\frac{B^2R^2}{\epsilon^2}\right)$  number of iterations or subgradients. Strongly Convex and Lipschitz Problem

## We now consider an even nicer problem class: $f(\mathbf{x})$

is  $\mu$ -strongly convex on X with  $\mu > 0$ :

$$f(\mathbf{x}) \ge f(\mathbf{y}) + \nabla f(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y}) + \frac{\mu}{2} ||\mathbf{x} - \mathbf{y}||_2^2. \quad \forall \mathbf{x}, \mathbf{y} \in X$$

# Lemma 5.11 Descent Lemma

$$\|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2 \le (1 - \mu \gamma_t) \|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - 2\gamma_t (f(\mathbf{x}_t) - f^*) + \gamma_t^2 \|\mathbf{g}_t\|_2^2$$

# Thm 5.12

Let f be  $\mu$ -strongly convex and B-Lipschitz conti**nuous** on X, then with  $\gamma_t = \frac{2}{u(t+1)}$ , we have

$$\min_{1 \le t \le T} f(\mathbf{x}_t) - f^* \le \frac{2B^2}{\mu \cdot (T+1)}$$

## Summary of Subgradient Method

	Cvx	Strongly C
Convergence rate	$O\left(\frac{B\cdot R}{\sqrt{t}}\right)$	$O\left(\frac{B^2}{\mu t}\right)$
Subgrad complexity	$O\left(\frac{B\cdot R}{\epsilon^2}\right)$	$O\left(\frac{B^2}{\mu\epsilon}\right)$

$$B := \sup_{\mathbf{x} \in X} \frac{|f(\mathbf{x}) - f(\mathbf{y})|}{\|\mathbf{x} - \mathbf{y}\|_2}, R := \max_{\mathbf{x}, \mathbf{y} \in X} \|\mathbf{x} - \mathbf{y}\|_2$$

# Subgradient Descent vs. Gradient Descent

Setting	Algo	Cvx	Strongly Cv
Nonsmooth	Subgrad	$O\left(\frac{B\cdot R}{\sqrt{t}}\right)$	$O\left(\frac{B^2}{\mu t}\right)$
Smooth	GD	$O\left(\frac{L \cdot R^2}{t}\right)$	$O\left(\left(1-\frac{\mu}{L}\right)^t\right)$
	AGD	$O\left(\frac{L \cdot R^2}{t^2}\right)$	$O\left(\left(1-\sqrt{\frac{\mu}{L}}\right)^{\frac{\mu}{L}}\right)$

# **Lower Complexity Bound for Nonsmooth Cvx Opt**

In the worst case, the sublinear rates  $O(1/\sqrt{t})$  and O(1/t) for convex and strongly convex Lipschitz problems cannot be improved, for algorithms using only subgradient oracles. Subgradient descent is "optimal"for such problem classes. Thm 5.13 (Nemirovski & Yudin, 1983)

For any  $1 \le t \le d$ ,  $\mathbf{x}_1 \in \mathbb{R}^d$ , there exists a B-Lipschitz continuous and convex function f, a convex set Xwith diameter R, such that for any first-order method that generates:

$$\mathbf{x}_t \in \mathbf{x}_1 + \operatorname{span}(\mathbf{g}_1, \dots, \mathbf{g}_{t-1}), \mathbf{g}_i \in \partial f(\mathbf{x}_i), i = 1, \dots, t-1$$

We have 
$$\min_{1 \le s \le t} f(\mathbf{x}_s) - f^* \ge \frac{B \cdot R}{4(1 + \sqrt{t})}$$
  
6. Stochastic Optimization

# **General Stochastic Optimization (SO) Problem**

$$\min_{\mathbf{x} \in \mathbb{R}^d} F(\mathbf{x}) := \mathbb{E}_{\boldsymbol{\xi}}[f(\mathbf{x}, \boldsymbol{\xi})]$$

- $\xi$  is a random vector with support  $\Xi \subset \mathbb{R}^m$  and
- For simplicity, assume  $f(\mathbf{x}, \xi)$  is continuously differentiable for any  $\xi \in \Xi$ .

#### **Finite Sum Problem**

$$\min_{\mathbf{x} \in \mathbb{R}^d} F(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x})$$

 $F(\mathbf{x}) = \mathbb{E}_{\xi} | f_{\xi}(\mathbf{x}) |$ , where  $\xi$  is uniformly distributed over  $\{1, 2, ..., n\}$ .

Pros: (1) Faster, (2) Memory efficient, (3) Avoid overfitting, help generalization.

Cons: (1) Lack of guarantee (2) Stuck at local solution, (3) Require strong assumptions

## **SGD for Finite Sum Problem**

Sample  $i_t \in [n]$  uniformly at random

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \nabla f_{i_t} \left( \mathbf{x}_t \right)$$

# Unbiasedness: $\mathbb{E}_{i_t} \left[ \nabla f_{i_t}(\mathbf{x}) \right] = \frac{1}{n} \sum_{i=1}^n \nabla f_i(\mathbf{x}) = \nabla F(\mathbf{x})$

# Each iteration is $\mathcal{O}(n)$ cheaper than full GD.

#### **Vanilla Analysis of Finite Sum Problem** If *i* is chosen at step *t*, then we have

$$\frac{\nabla f_i(\mathbf{x}_t)^{\top}(\mathbf{x}_t - \mathbf{x}^*)}{= \frac{\gamma_t}{2} \|\nabla f_i(\mathbf{x}_t)\|_2^2 + \frac{1}{2\gamma_t} (\|\mathbf{x}_t - \mathbf{x}^*\|_2^2 - \|\mathbf{x}_{t+1} - \mathbf{x}^*\|_2^2)}$$

# **SGD for General Stochastic Optimization**

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t)$$
, where  $\boldsymbol{\xi}_t \stackrel{iid}{\sim} P(\boldsymbol{\xi})$ 

# **Boundedness of Stochastic Gradients**

Let  $F(\mathbf{x}) = \mathbb{E}[f(\mathbf{x}, \boldsymbol{\xi})]$ , where  $f(\mathbf{x}, \boldsymbol{\xi})$  is convex and L-smooth for any realization of  $\xi$ . Define  $\mathbf{x}^* =$  $\operatorname{argmin}_{\mathbf{x}} F(\mathbf{x})$ . Then we have

$$\mathbb{E}\left[\left\|\nabla f(\mathbf{x}, \xi) - \nabla f(\mathbf{x}^*, \xi)\right\|_2^2\right] \le 2L\left[F(\mathbf{x}) - F(\mathbf{x}^*)\right]$$

$$\mathbb{E}\left[\left\|\nabla f(\mathbf{x},\xi)\right\|_{2}^{2}\right] \leq 4L\left[F(\mathbf{x}) - F(\mathbf{x}^{*})\right] + 2\mathbb{E}\left[\left\|\nabla f(\mathbf{x}^{*},\xi)\right\|_{2}^{2}\right]$$

#### (Proof see Hw6 Ex1&2) **Unbiasedness:** $\mathbb{E}[\nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t) | \mathbf{x}_t] = \nabla F(\mathbf{x}_t)$ under

mild regularity conditions We always assume stochastic gradient is unbiased.

Stepsize (or Learning Rate) · If use fixed stepsize for SGD as in GD, SGD will

Note SGD is **not** a monotonic descent method.

- not converge to the optimal solution (almost sure-
- Stepsize should decrease to  $0, \gamma_t \to 0$
- For example, use polynomial rate  $\gamma_t = \mathcal{O}(t^{-a})$ with some a > 0• In practice, use the form  $\gamma_t = \frac{\gamma_0}{1+\beta t}$  and tune hy-
- perparameters  $\gamma_0, \beta$
- In deep learning, often adopt step decay drop the learning rate by a factor every few epochs.

#### **Simple Improvements of SGD Mini-batch SGD**

Use b random samples to construct gradient estima-

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \cdot \frac{1}{b} \sum_{j \in J, |J| = b} \nabla f\left(\mathbf{x}_t, \xi_j\right)$$

## SGD with iterate averaging

$$\overline{\mathbf{x}}_t = \frac{1}{t} \sum_{\tau=1}^t \mathbf{x}_{\tau}$$

Averaging and mini-batch sampling can help reduce Still, SGD can be very sensitive to the choice of

#### stepsize. **Limitations of SGD**

- learning rate tuning
- uniform learning rate for all coordinates

#### **Convergence for Stochastic Convex Problems** Thm 6.1 (Convex, weighted averaging)

Suppose  $F(\mathbf{x})$  is **convex** and  $\mathbb{E}\left[\|\nabla f(\mathbf{x},\xi)\|_2^2\right] \leq B^2, \forall \mathbf{x}$ . Then SGD satisfies that

$$\mathbb{E}\left[F(\hat{\mathbf{x}}_T) - F(\mathbf{x}^*)\right] \le \frac{R^2 + B^2 \sum_{t=1}^T \gamma_t^2}{2\sum_{t=1}^T \gamma_t^2}$$

where  $\hat{\mathbf{x}}_T := \sum_{t=1}^T \gamma_t \mathbf{x}_t / \sum_{t=1}^T \gamma_t$  and  $||\mathbf{x}_1 - \mathbf{x}^*||_2 \le R$ .

- If  $\gamma_t \equiv \frac{R}{R_0/T}$ ,  $\mathbb{E}[F(\hat{\mathbf{x}}_T) F(\mathbf{x}^*)] = \mathcal{O}(\frac{BR}{\sqrt{T}})$ .
- This further implies the  $\mathcal{O}(1/\epsilon^2)$  sample complexity required by SGD.

### Thm 6.2 (Strong convex, diminishing stepsize, last $F(\mathbf{x})$ is $\mu$ -strongly convex and Assume

 $\mathbb{E}[\|\nabla f(\mathbf{x},\xi)\|_2^2] \leq B^2, \forall \mathbf{x}, \text{ then SGD with } \gamma_t =$  $\frac{\gamma}{t} \left( \gamma > \frac{1}{2u} \right)$  satisfies

$$\mathbb{E}\left[\left\|\mathbf{x}_{t}-\mathbf{x}^{*}\right\|_{2}^{2}\right] \leq \frac{C(\gamma)}{t}$$

where  $C(\gamma) = \max \left\{ \frac{\gamma^2 B^2}{2u\gamma - 1}, ||\mathbf{x}_1 - \mathbf{x}^*||_2^2 \right\}$ • If F is also L-smooth, this further implies that

- $\mathbb{E}\left[F\left(\mathbf{x}_{t}\right) f\left(\mathbf{x}^{*}\right)\right] = \mathcal{O}\left(\frac{L \cdot C(\gamma)}{t}\right).$ • The sample complexity required by SGD is  $\mathcal{O}(1/\epsilon)$
- in this case.

# SGD under Constant Stepsize (Thm 5.3)

Assume that (1)  $F(\mathbf{x}) := \mathbb{E}[f(\mathbf{x}, \boldsymbol{\xi})]$  is  $\mu$ -strongly convex and L-smooth; (2) The unbiased estimator satisfies that for all x:

$$\mathbb{E}\left[\left\|\nabla f(\mathbf{x}, \boldsymbol{\xi})\right\|_{2}^{2}\right] \leq \sigma^{2} + c\left\|\nabla F(\mathbf{x})\right\|_{2}^{2}$$

Under the above assumption, SGD with  $\gamma_t = \gamma \leq \frac{1}{L_c}$ 

$$\mathbb{E}\left[F\left(\mathbf{x}_{t}\right) - F\left(\mathbf{x}^{*}\right)\right] \leq \frac{\gamma L \sigma^{2}}{2\mu} + (1 - \mu \gamma)^{t-1} \left(F\left(\mathbf{x}_{1}\right) - F\left(\mathbf{x}^{*}\right)\right)$$

- With constant stepsize, SGD converges linearly to a neighborhood around x\*.
- Accuracy-convergence trade-off: Smaller stepsize  $\gamma$  implies better solution but slower rate.
- Strong Growth Condition: when  $\sigma^2 = 0$ , i.e.,  $\mathbb{E}\left[\|\nabla f(\mathbf{x}, \boldsymbol{\xi})\|_{2}^{2}\right] \leq c\|\nabla F(\mathbf{x})\|_{2}^{2}$ , SGD with constant stepsize converges to the global optimum at a linear rate.
- Consider  $F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{x})$ , strong growth condition implies interpolation: at optimal solution  $\mathbf{x}^*$ ,  $\nabla f_i(\mathbf{x}^*) = 0$ ,  $\forall i$ .
- Strong growth condition holds when F is smooth and satisfies PL inequality.
- Examples: linear regression or overparametrized neural network in the realizable case.

# **SGD Summary**

	Cvx	Strongly Cvx		
Convergence rate	$O\left(\frac{1}{\sqrt{t}}\right)$	$O\left(\frac{1}{t}\right)$		
Sample complexity	$O\left(\frac{1}{\epsilon^2}\right)$	$O\left(\frac{1}{\epsilon}\right)$		

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# Lower Complexity Bound for Stochastic Optimizati-In the worst case, the sample complexity $\mathcal{O}(1/\epsilon^2)$

problems cannot be improved, for algorithms using only stochastic oracles. Stochastic Oracle: given input x, stochastic oracle returns  $G(\mathbf{x}, \boldsymbol{\xi})$  such that

and  $\mathcal{O}(1/\epsilon)$  for convex and strongly convex Lipschitz

$$\mathbb{E}[G(\mathbf{x}, \xi)] \in \partial f(\mathbf{x}) \text{ and } \mathbb{E}[||G(\mathbf{x}, \xi)||_p^2] \le M^2$$

for some positive constant M and some  $p \in [1, \infty]$ . SGD is **optimal** for such problem classes.

# Popular Variants of SGD

Momentum SGD 
$$\int \mathbf{m}_t = \alpha \mathbf{m}_{t-1} + (1-\alpha) \nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t)$$

 $\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \mathbf{m}_t$ 

### AdaGrad

$$\begin{cases} \mathbf{v}_t &= \mathbf{v}_{t-1} + \nabla f\left(\mathbf{x}_t, \boldsymbol{\xi}_t\right)^{\odot 2} \\ \mathbf{x}_{t+1} &= \mathbf{x}_t - \frac{\gamma_0}{\epsilon + \sqrt{\mathbf{v}_t}} \odot \nabla f\left(\mathbf{x}_t, \boldsymbol{\xi}_t\right) \end{cases}$$

## **RMSProp**

$$\begin{cases} \mathbf{v}_t &= \beta \mathbf{v}_{t-1} + (1-\beta) \nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t)^{\odot 2} \\ \mathbf{x}_{t+1} &= \mathbf{x}_t - \frac{\gamma_0}{\varepsilon + \sqrt{\mathbf{v}_t}} \odot \nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t) \end{cases}$$

ADAM ≈ RMSProp + Momentum

$$\begin{cases} \mathbf{v}_t &= \beta \mathbf{v}_{t-1} + (1-\beta) \nabla f \left(\mathbf{x}_t, \boldsymbol{\xi}_t\right)^{\odot 2} \\ \mathbf{m}_t &= \alpha \mathbf{m}_{t-1} + (1-\alpha) \nabla f \left(\mathbf{x}_t, \boldsymbol{\xi}_t\right) \\ \mathbf{x}_{t+1} &= \mathbf{x}_t - \frac{\gamma_0}{\varepsilon + \sqrt{\overline{\mathbf{v}}_t}} \odot \tilde{\mathbf{m}}_t \end{cases}$$

- Exponential decay of previous information  $\mathbf{m}_t, \mathbf{v}_t$ .
- Note  $\tilde{\mathbf{v}}_t = \frac{\mathbf{v}_t}{1-\beta^t}$  and  $\tilde{\mathbf{m}}_t = \frac{\mathbf{m}_t}{1-\alpha^t}$  are bias-corrected
- In practice,  $\alpha$  and  $\beta$  are chosen to be close to 1.

### **Generic Adaptive Scheme**

$$\mathbf{g}_{t} = \nabla f \left( \mathbf{x}_{t}, \boldsymbol{\xi}_{t} \right)$$

$$\mathbf{m}_{t} = \phi_{t} \left( \mathbf{g}_{1}, \dots, \mathbf{g}_{t} \right)$$

$$\mathbf{V}_{t} = \psi_{t} \left( \mathbf{g}_{1}, \dots, \mathbf{g}_{t} \right)$$

$$\hat{\mathbf{x}}_{t} = \mathbf{x}_{t} - \alpha_{t} \mathbf{V}_{t}^{-1/2} \mathbf{m}_{t}$$

$$\mathbf{x}_{t+1} = \underset{\mathbf{x} \in X}{\operatorname{argmin}} \left\{ \left( \mathbf{x} - \hat{\mathbf{x}}_{t} \right)^{T} \mathbf{V}_{t}^{1/2} \left( \mathbf{x} - \hat{\mathbf{x}}_{t} \right) \right\}$$

- SGD:  $\phi_t(\mathbf{g}_1,...,\mathbf{g}_t) = \mathbf{g}_t, \quad \psi_t(\mathbf{g}_1,...,\mathbf{g}_t) = \mathbf{I}$
- AdaGrad:  $\phi_t(\mathbf{g}_1,...,\mathbf{g}_t) = \mathbf{g}_t, \quad \psi_t(\mathbf{g}_1,...,\mathbf{g}_t) =$  $\operatorname{diag}(\sum_{\tau=1}^t \mathbf{g}_{\tau}^2)$

• Adam:  $\phi_t(\mathbf{g}_1,...,\mathbf{g}_t) = (1-\beta_1)\sum_{\tau=1}^t \beta_1^{t-\tau}\mathbf{g}_{\tau}$ ,  $\psi_t(\mathbf{g}_1,\ldots,\mathbf{g}_t) = (1-\beta_2)\operatorname{diag}\left(\sum_{\tau=1}^t \beta_2^{t-\tau}\mathbf{g}_\tau^2\right).$  In other words,  $\mathbf{m}_t = \beta_1 \mathbf{m}_{t-1} + (1 - \beta_1) \mathbf{g}_t, \mathbf{V}_t =$  $\beta_2 \mathbf{V}_{t-1} + (1 - \beta_2) \operatorname{diag}(\mathbf{g}_t^2).$ 7. Variance-reduced Stochastic Methods The Non-Convergence of Adam

**Counterexample**: consider a one-dim problem:

$$X = [-1, 1], f(x, \xi) = \begin{cases} Cx, & \text{if } \xi = 1\\ -x, & \text{if } \xi = 0 \end{cases}$$
$$\mathbb{P}(\xi = 1) = p = \frac{1 + \delta}{C + 1}$$

- Here  $F(x) = \mathbb{E}[f(x,\xi)] = \delta x$  and  $x^* = -1$ .
- Adam step is  $x_{t+1} = x_t \gamma_0 \Delta_t$  with  $\Delta_t =$  $\sqrt{\beta v_t + (1-\beta)g_t^2}$
- For large enough C > 0, one can show  $\mathbb{E}[\Delta_t] \leq 0$ . · Adam steps keep drifting away from the optimal
- solution  $x^* = -1$ . SGD vs. GD for Finite Sum Problem

#### Complexity for smooth and strongly-convex problems: $\kappa := L/\mu$ .

iter complexity | per-iter cost  $\mathcal{O}(\kappa \cdot \ln \frac{1}{2})$ GD  $\mathcal{O}(n)$ 

300	$O(\overline{\epsilon})$		J(1)		$(\overline{\epsilon})$
• GD c	onverges faster	but with	expensiv	e iter	cost.

- SGD converges slowly but with cheap iter cost. • SGD is more appealing for large *n* and moderate
- accuracy  $\epsilon$ .

#### SGD vs. GD vs. VR Methods Algo | # of Iterations | Per-iteration Cost $O(\kappa \log \frac{1}{\epsilon})$ O(n) $O\left(\frac{\kappa}{\epsilon}\right)$ SGD O(1) $O((n+\kappa)\log\frac{1}{\epsilon})$ O(1)

**Classical Variance Reduction Techniques** 

SCD

$$\min_{\mathbf{x} \in \mathbb{R}^d} F(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x})$$

Mini-batching: Use the average of gradients from a random subset

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \frac{1}{|B_t|} \sum_{i \in B_t} \nabla f_i\left(\mathbf{x}_t\right)$$

Note: VR comes at a computational cost. Momentum: add momentum to the gradient step

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \hat{\mathbf{m}}_t$$
, where  $\hat{\mathbf{m}}_t = c \cdot \sum_{\tau=1}^t \alpha^{t-\tau} \nabla f_{i_\tau}(\mathbf{x}_\tau)$ 

Note: Here  $\mathbf{m}_t$  is the weighted average of the past stochastic gradients.

**Modern Variance Reduction Technique** Suppose X is positively correlated with Y and we

can compute  $\mathbb{E}[Y]$ . **Point Estimator:** 

 $\alpha = 1, Y = \mathbf{v}_{i_{+}}$ 

$$\hat{\Theta}_{\alpha} = \alpha(X - Y) + \mathbb{E}[Y], \quad (0 \le \alpha \le 1)$$

$$\mathbb{E}[\hat{\Theta}_{\alpha}] = \alpha \mathbb{E}[X] + (1 - \alpha)\mathbb{E}[Y]$$

$$\mathbb{V}[\hat{\Theta}_{\alpha}] = \alpha^{2}(\mathbb{V}[X] + \mathbb{V}[Y] - 2\operatorname{Cov}[X, Y])$$

If cov is sufficiently large, then  $\mathbb{V}\left[\hat{\Theta}_{\alpha}\right] \leq \mathbb{V}[X]$ . **Variance Reduction Techniques for Finite Sum Pro-**Goal: estimate  $\theta = \nabla F(\mathbf{x}_t), X = \nabla f_{i_t}(\mathbf{x}_t)$ 

• **SGD**:  $\mathbf{g}_t = \nabla f_{i_t}(\mathbf{x}_t) [\alpha = 1, Y = 0]$ 

$$\left[\alpha = \frac{1}{n}, Y = \mathbf{v}_{i_t}\right]$$
• SAGA:  $\mathbf{g}_t = \left(\nabla f_{i_t}(\mathbf{x}_t) - \mathbf{v}_{i_t}\right) + \frac{1}{n} \sum_{i=1}^{n} \mathbf{v}_i$ 

• SAG:  $\mathbf{g}_t = \frac{1}{n} \left( \nabla f_{i_t}(\mathbf{x}_t) - \mathbf{v}_{i_t} \right) + \frac{1}{n} \sum_{i=1}^n \mathbf{v}_i$ 

Here  $\{\mathbf{v}_i, i = 1, ..., n\}$  are the past stored gradients for each component.

total cost 
$$\mathcal{O}(n\kappa \ln \frac{1}{\epsilon})$$
 SVRG:  $\mathbf{g}_t = \nabla f_{i_t}(\mathbf{x}_t) - \nabla f_{i_t}(\tilde{\mathbf{x}}) + \nabla F(\tilde{\mathbf{x}})$   $\left[\alpha = 1, Y = \nabla f_{i_t}(\tilde{\mathbf{x}})\right]$ 

Idea: keep track of the average of  $\mathbf{v}_i$  as an estimate of the full gradient

$$\mathbf{g}_{t} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{v}_{i}^{t} \quad \approx \quad \frac{1}{n} \sum_{i=1}^{n} \nabla f_{i}\left(\mathbf{x}_{t}\right) = \nabla F\left(\mathbf{x}_{t}\right)$$

The past gradients are updated as:

Stochastic Average Gradient (SAG)

$$\mathbf{v}_i^t = \begin{cases} \nabla f_{i_t}(\mathbf{x}_t), & \text{if } i = i_t \\ \mathbf{v}_i^{t-1}, & \text{if } i \neq i_t \end{cases}$$

Equivalently, we have

$$\mathbf{g}_{t} = \mathbf{g}_{t-1} - \frac{1}{n} \underbrace{\mathbf{v}_{i_{t}}^{t-1}}_{Y} + \frac{1}{n} \underbrace{\nabla f_{i_{t}}(\mathbf{x}_{t})}_{X}$$

 $\mathbf{x}_{t+1} = \mathbf{x}_t - \frac{\gamma}{n} \sum_{i=1}^n \mathbf{v}_i^t,$ where  $\mathbf{v}_{i}^{t} = \begin{cases} \nabla f_{i_{t}}(\mathbf{x}_{t}), & \text{if } i = i_{t} \\ \mathbf{v}_{i}^{t-1}, & \text{otherwise} \end{cases}$ 

Biased gradient; Cheap iteration cost; O(nd) memory cost; Hard to analyze.

- Linear convergence: The first stochastic methods to enjoy linear rate using a constant stepsize for strongly-convex and smooth objectives.
- Memory cost: O(n) times higher than SGD/SVRG
- Per-iteration cost: one gradient evaluation • Total complexity:  $O((n + \kappa_{\max}) \log(\frac{1}{\epsilon}))$

**SAGA** 

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma \left[ \left( \nabla f_{i_t} \left( \mathbf{x}_t \right) - \mathbf{v}_{i_t}^{t-1} \right) + \frac{1}{n} \sum_{i=1}^{n} \mathbf{v}_i^{t-1} \right]$$

- Unbiased update, while SAG is biased
- Same  $\mathcal{O}(nd)$  memory cost as SAG
- Similar linear convergence rate as SAG

# Stochastic Variance Reduced Gradient (SVRG)

**Intuition**: the closer  $\tilde{\mathbf{x}}$  is to  $\mathbf{x}_t$ , the smaller the variance of the gradient estimator

$$\mathbb{E}\left[\left\|\mathbf{g}_{t} - \nabla F\left(\mathbf{x}_{t}\right)\right\|^{2}\right] \leq \mathbb{E}\left[\left\|\nabla f_{i_{t}}\left(\mathbf{x}_{t}\right) - \nabla f_{i_{t}}(\tilde{\mathbf{x}})\right\|^{2}\right]$$

$$\leq L_{\max}^{2} \left\|\mathbf{x}_{t} - \tilde{\mathbf{x}}\right\|^{2}$$

# Two-loop structure:

- Outer loop: update reference point and compute its full gradient at O(n) cost
- Inner loop: update iterates with variance-reduced gradient for *m* steps
- Total of O(n+2m) component gradient evaluations at each epoch

#### Compare to SAG/SAGA Pro: Cheap memory cost, no need to store past gra-

dients or past iterates Con: More parameter tuning, two gradient computation per iteration

Thm 7.1 Convergence of SVRG

Assume each  $f_i(\mathbf{x})$  is convex and  $L_i$ -smooth,  $F(\mathbf{x})$  is  $\mu$ strongly convex. Assume m is sufficiently large and  $\eta < \frac{1}{2L_{\max}}$  such that  $\rho = \frac{1}{\mu\eta(1-2\eta L_{\max})m} + \frac{2\eta L_{\max}}{1-2\eta L_{\max}}$ 1. then

$$\mathbb{E}\left[F\left(\tilde{\mathbf{x}}^{s}\right) - F\left(\mathbf{x}^{*}\right)\right] \leq \rho^{s} \left[F\left(\tilde{\mathbf{x}}^{0}\right) - F\left(\mathbf{x}^{*}\right)\right]$$

**Linear convergence:** choose  $m = \mathcal{O}(\frac{L_{\text{max}}}{u}), \eta =$  $\mathcal{O}\left(\frac{1}{L_{\max}}\right)$  such that  $\rho \in \left(0, \frac{1}{2}\right)$ . Total complexity:

$$\mathcal{O}\left((2m+n)\log\frac{1}{\epsilon}\right) = \mathcal{O}\left(\left(n + \frac{L_{\max}}{\mu}\right)\log\frac{1}{\epsilon}\right)$$

## **Lemma 7.2 Property of Smoothness**

Let  $F(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} f_i(\mathbf{x})$ , where each  $f_i : \mathbb{R}^d \to \mathbb{R}$  is a convex and  $L_i$ -smooth function and F has a global minimum  $\mathbf{x}^*$ . Let  $L_{\text{max}} = \max\{L_1, \dots, L_n\}$ . Then, for any  $\mathbf{x} \in \mathbb{R}^d$ 

$$\frac{1}{n} \sum_{i=1}^{n} \left\| \nabla f_i(\mathbf{x}) - \nabla f_i(\mathbf{x}^*) \right\|_2^2 \le 2L_{\max} \left[ F(\mathbf{x}) - F(\mathbf{x}^*) \right]$$

Lemma 7.3 Bound of Variance  $\phi_M$  is defined by  $\tilde{\mathbf{x}}, \mathbf{x}_t \in \mathbb{R}^d$ . Denote  $\mathbf{g}_t = \nabla f_{i_t}(\mathbf{x}_t) - \nabla f_{i_t}(\tilde{\mathbf{x}}) + \nabla F(\tilde{\mathbf{x}})$ , whe-

# re $i_t$ is sampled uniformly from $\{1, ..., n\}$ . Then

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$$\mathbb{E}\left[\|\mathbf{g}_{t}\|_{2}^{2}\right] \leq 4L_{\max}\left[F\left(\mathbf{x}_{t}\right) - F\left(\mathbf{x}^{*}\right) + F(\tilde{\mathbf{x}}) - F\left(\mathbf{x}^{*}\right)\right]$$

### f is called **concave** if -f is convex. For all **x**, the graph of a differentiable concave func-

tion is below the tangent hyperplane at x.  $\Rightarrow$  concave functions are smooth with L = 0... but boring from an optimization point of view (no global

minimum), gradient descent runs off to infinity   
**Lemma 8.1 Bounded Hessians** 
$$\Rightarrow$$
 **smooth**  
Let  $f: \text{dom}(f) \to \mathbb{R}$  be twice differentiable, with

$$X \subseteq \text{dom}(f)$$
 a convex set, and  $\|\nabla^2 f(\mathbf{x})\| \le L$  for all  $\mathbf{x} \in X$ , where  $\|\cdot\|$  is spectral norm. Then  $f$  is smooth with parameter  $L$  over  $X$ .

Examples:

• all quadratic functions  $f(\mathbf{x}) = \mathbf{x}^{\top} A \mathbf{x} + \mathbf{b}^{\top} \mathbf{x} + c$ 

• 
$$f(x) = \sin(x)$$
 (many global minima)

# convex) functions

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be differentiable with a global minimum  $\mathbf{x}^*$ ; furthermore, suppose that f is smooth

nimum 
$$x^*$$
; furthermore, suppose that  $f$  is smooth with parameter  $L$  according to Definition 3.2. Choosing stepsize  $\gamma := \frac{1}{L}$ . Gradient descent yields

$$\frac{1}{T} \sum_{t=0}^{T-1} \|\nabla f(\mathbf{x}_t)\|^2 \le \frac{2L}{T} \left( f(\mathbf{x}_0) - f(\mathbf{x}^*) \right), \quad T > 0$$
.
In particular,  $\|\nabla f(\mathbf{x}_t)\|^2 \le \frac{2L}{T} \left( f(\mathbf{x}_0) - f(\mathbf{x}^*) \right)$  for so-

me  $t \in \{0, ..., T-1\}$ . Corollary of Thm 8.2 Thm 8.2 implies that

$$\lim_{t\to\infty} \|\nabla f(\mathbf{x}_t)\|^2 = 0.$$

### Lemma 8.3 No overshooting In the smooth setting, and with stepsize 1/L, gra-

# **Local Optimality Problem** Let $\mathcal{F}$ be a class of functions from $\mathbb{R}^n$ to $\mathbb{R}$ .

dient descent cannot overshoot, i.e. pass a critical

The problem LocMin( $\mathcal{F}$ ) is to decide whether **0** is a local minimum of a given function  $\phi \in \mathcal{F}$ .

class 
$$\mathcal{F} := \{\phi_{\mathbf{M}} : \mathbf{M} \text{ symmetric}\}$$
, where the function  $\phi_M$  is defined by 
$$\phi_M(\mathbf{x}) = \left(\mathbf{x}^2\right)^\top \mathbf{M} \left(\mathbf{x}^2\right)$$

The problem LOCMIN( $\mathcal{F}$ ) is coNP-complete for the

$$\phi_M(\mathbf{x}) = (\mathbf{x}^2)^{\top} \mathbf{M}(\mathbf{x}^2)$$
 with  $\mathbf{x}^2 = (x_1^2, x_2^2, \dots, x_n^2)$  Proof outline:

0 is a local minimum iff the matrrix M is copositive. Deciding whether **M** is copositive is coNP-complete. **Copositive matrices** 

# **0** is a local minimum of $(\mathbf{x}^2)^{\top} \mathbf{M} (\mathbf{x}^2)$ iff $\mathbf{x}^{\top} \mathbf{M} \mathbf{x} \ge 0$ for all $x \ge 0$ .

Thm (Murty and Kabadi [MK87])

A matrix M satisfying  $\mathbf{x}^{\top} \mathbf{M} \mathbf{x} \geq 0$  for all  $\mathbf{x} \geq \mathbf{0}$  is called **copositive**. If M is positive semidefinite  $(\mathbf{x}^{\top} M \mathbf{x} \ge 0 \text{ for all } \mathbf{x})$ , then **M** is copositive. The converse is false.

0 is a local minimum  $\Leftrightarrow$   $(\mathbf{x}^2)^{\top} \mathbf{M}(\mathbf{x}^2) \ge 0$  for all  $\mathbf{x}$  in some neighborhood of **Frank-Wolfe Algorithm**  $\Leftrightarrow \mathbf{x}^{\top} \mathbf{M} \mathbf{x} \ge 0$  for all  $\mathbf{x} \ge \mathbf{0}$  in some neighborhood of  $\mathbf{0}$  dependent) stepsizes  $\gamma_t \in [0,1]$ , repeat the following

**Def 8.4** 
$$c$$
**-balanced**  
Let  $x > 0$  (componentwise), and let  $c \ge 1$  be a real number.  $x$  is called  $c$ **-balanced** if  $x_i \le cx_j$  for all  $1 \le i, j \le d$ .

Any initial iterate  $\mathbf{x}_0 > \mathbf{0}$  is c-balanced for some (pos-

sibly large) c. **Lemma 8.5 Balanced iterates** Let  $\mathbf{x} > \mathbf{0}$  be *c*-balanced with  $\prod_k x_k \le 1$ . Then for any stepsize  $\gamma > 0$ ,  $\mathbf{x}' := \mathbf{x} - \gamma \nabla f(\mathbf{x})$  satisfies  $\mathbf{x}' \geq \mathbf{x}$ (componentwise) and is also *c*-balanced.

Suppose that 
$$\mathbf{x} > \mathbf{0}$$
 is *c*-balanced. Then for any  $I \subseteq \{1, ..., d\}$ , we have 
$$\left(\frac{1}{c}\right)^{|I|} \left(\prod x_k\right)^{1-|I|/d} \leq \prod x_k \leq c^{|I|} \left(\prod x_k\right)^{1-|I|/d}$$

# Lemma 8.7

 $\Leftrightarrow \mathbf{x}^{\top} \mathbf{M} \mathbf{x} > 0$  for all  $\mathbf{x} > \mathbf{0}$ 

Let  $\mathbf{x} > \mathbf{0}$  be *c*-balanced with  $\prod_k x_k \leq 1$ . Then  $\|\nabla^2 f(\mathbf{x})\|_2 \le \|\nabla^2 f(\mathbf{x})\|_E \le 3dc^2$ 

where 
$$\|\cdot\|_F$$
 is the Frobenius norm and  $\|\cdot\|_2$  the

spectral norm. Let x > 0 be c-balanced with  $\prod_k x_k < 1, L = 3dc^2$ . Let

 $\gamma := 1/L$ . We already know from Lemma 8.5 that  $\mathbf{x}' := \mathbf{x} - \gamma \nabla f(\mathbf{x}) \ge \mathbf{x}$  is *c*-balanced. Furthermore, f is smooth with parameter L over the line segment connecting x and x'. Lemma 8.3 (no overshooting) then also yields  $\prod_k x'_k \le 1$ .

**Thm 8.9 Convergence of Balanced Iterates** Let  $c \ge 1$  and  $\delta > 0$  such that  $\mathbf{x}_0 > \mathbf{0}$  is c-balanced with  $\delta \leq \prod_k (\mathbf{x}_0)_k < 1$ . Choosing stepsize  $\gamma = \frac{1}{3dc^2}$ ,

gradient descent satisfies  $f(\mathbf{x}_T) \le \left(1 - \frac{\delta^2}{3c^4}\right)^T f(\mathbf{x}_0), \quad T \ge 0$ 

The sequence  $(\mathbf{x}_T)_{T>0}$  of iterates in Thm 8.9 converges to a an optimal solution  $x^*$ .

9. The Frank-Wolfe Algorithm **Linear minimization oracle** Given  $\mathbf{g} \in \mathbb{R}^d$ ,  $LMO_X(\mathbf{g}) := \operatorname{argmin} \mathbf{g}^{\top} \mathbf{z}$ 

is any minimizer of the linear function 
$$\mathbf{g}^{\mathsf{T}}\mathbf{z}$$
 over  $X$ . Lemma 9.1 We assume that a minimizer exists whenever we apply the oracle. If  $X$  is closed and bounded, this is

ply the oracle. If *X* is closed and bounded, this is guaranteed. Given an initial feasible point  $\mathbf{x}_0 \in X$ , and (time-

 $\mathbf{s} := \mathrm{LMO}_{X} \left( \nabla f \left( \mathbf{x}_{t} \right) \right)$ 

 $\mathbf{x}_{t+1} := (1 - \gamma_t)\mathbf{x}_t + \gamma_t \mathbf{s}$ 

Let 
$$\mathbf{y} := \mathbf{x}_{t+1} = \mathbf{x} + \gamma(\mathbf{s} - \mathbf{x})$$
, then 
$$\frac{1}{v^2} ||\mathbf{y} - \mathbf{x}||^2 = ||\mathbf{s} - \mathbf{x}||^2$$

# The Frank-Wolfe algorithm is particularly useful

for t = 0, 1, ...:

nice set of points A (the atoms, or extreme points), • LMO<sub>X</sub>( $\mathbf{g}$ ) = argmin<sub> $\mathbf{z} \in X$ </sub>  $\mathbf{g}^{\mathsf{T}} \mathbf{z}$  is always attained by

when *X* is the convex hull of a finite or otherwise

• This may significantly simplify the search for  $s = LMO_X(g)$ . **Example: Spectahedron** 

#### Hazan's algorithm: an application of the Frank-Wolfe algorithm to semidefinite programming. $LMO_X(\mathbf{G})$ :

argmin  $G \bullet Z$  $Tr(\mathbf{Z}) = 1$ subject to

positive semidefinite matrices  $\mathbf{Z} \in \mathbb{R}^{d \times d}$  of trace 1. Spectahedron:  $X = \{ \mathbf{Z} \in \mathbb{R}^{d \times d} : \text{Tr}(\mathbf{Z}) = 1, \mathbf{Z} \succeq 0 \}$ 

• **G** is a symmetric matrix.

of *X* (which exists since *X* is closed and bounded). • Standard stepzise in the Frank-Wolfe algorithm:  $\gamma_t = 2/(t+2)$ . • We need to assume that *f* is smooth, but the smoo-

• A • B stands for the scalar product of two square

• The LMO is a semidefinite program itself, but of

a simple form that allows an explicit solution.

• Atoms: The matrices of the form  $zz^{\top}$  with  $z \in$ 

Need to show: every  $\mathbf{Z} \in X$  is a convex combination

• diagonalize:  $\mathbf{Z} = \mathbf{T}\mathbf{D}\mathbf{T}^{\top}$  where  $\mathbf{T}$  is orthogonal

• D's diagonal elements  $\lambda_1, \dots, \lambda_d$  are the (nonnega-

• Let **a**<sub>i</sub> be the *i*-th column of **T**. As **T** is orthogonal,

•  $\mathbf{Z} = \sum_{i=1}^{d} \lambda_i \mathbf{a}_i \mathbf{a}_i^{\mathsf{T}}$  is the desired convex combination of atoms.

Let  $\lambda_1$  be the smallest eigenvalue of **G**, and let  $\mathbf{s}_1$  be

a corresponding eigenvector of unit length. Then we

Duality gap:  $g(\mathbf{x}) := \nabla f(\mathbf{x})^{\top} (\mathbf{x} - \mathbf{s})$  for  $\mathbf{s} :=$ 

Suppose that the constrained minimization problem

 $\min\{f(\mathbf{x}): \mathbf{x} \in X\}$  has a minimizer  $\mathbf{x}^*$ . Let  $\mathbf{x} \in X$ .

 $g(\mathbf{x}) \ge f(\mathbf{x}) - f(\mathbf{x}^*)$ 

meaning that the duality gap is an upper bound for

Consider the constrained minimization problem

 $\min\{f(\mathbf{x}): \mathbf{x} \in X\}$  where  $f: \mathbb{R}^d \to \mathbb{R}$  is convex and smooth with parameter L, and set X is convex, clo-

sed and bounded (in particular, a minimizer  $x^*$  of f

over X exists, and all linear minimization oracles ha-

ve minimizers). With any  $\mathbf{x}_0 \in X$ , and with stepsizes

 $f(\mathbf{x}_T) - f(\mathbf{x}^*) \le \frac{2L \operatorname{diam}(X)^2}{T+1}, \quad T \ge 1$ 

where diam(X) :=  $\max_{\mathbf{x},\mathbf{y}\in X} ||\mathbf{x}-\mathbf{y}||$  is the diameter

 $\gamma_t = 2/(t+2)$ , the Frank-Wolfe algorithm yields

Thm 9.3 Convergence in  $\mathcal{O}(1/\varepsilon)$  steps

 $\mathbb{R}^d$ ,  $\|\mathbf{z}\| = 1$  (these are positive semidefinite of trace

matrices **A** and **B**,  $\mathbf{A} \bullet \mathbf{B} = \sum_{i,j} a_{ij} b_{ij}$ .

1 and hence in X).

and **D** is diagonal, of trace 1.

tive) eigenvalues of **Z**.

can choose LMO<sub>X</sub>(**G**) =  $\mathbf{s}_1 \mathbf{s}_1^{\top}$ .

we have  $\|\mathbf{a}_i\| = 1$ .

of atoms.

Lemma 9.2

the optimality gap.

**Lemma 9.4 Descent Lemma** For a step  $\mathbf{x}_{t+1} := \mathbf{x}_t + \gamma_t (\mathbf{s} - \mathbf{x}_t)$  with stepsize  $\gamma_t \in$ [0,1], it holds that

thness parameter L does not enter the stepsize.

 $f(\mathbf{x}_{t+1}) \le f(\mathbf{x}_t) - \gamma_t g(\mathbf{x}_t) + \gamma_t^2 \frac{L}{2} \|\mathbf{s} - \mathbf{x}_t\|^2$ where  $\mathbf{s} = \text{LMO}_X (\nabla f(\mathbf{x}_t))$ .

**Curvature Constant** Optimization for Data Science Yilei Tu, Page 9 of 14

### Stepsize variants Writing $h(\mathbf{x}) := f(\mathbf{x}) - f(\mathbf{x}^*)$ for the (unknown) opti-

mization gap at point **x**, and we have  $h(\mathbf{x}) \leq g(\mathbf{x})$ . Let  $C := \frac{L}{2} \operatorname{diam}(X)^2$ . Thm 9.3 can be written as

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) = h(\mathbf{x}_t) \le \frac{4C}{t+1}, \quad t \ge 1$$

# Line search stepsize $\gamma_t := \operatorname{argmin} f((1 - \gamma)\mathbf{x}_t + \gamma \mathbf{s})$

Let 
$$\mathbf{y}_{t+1}$$
 be the iterate obtained from  $\mathbf{x}_t$  with the standard stepsize  $\mu_t = 2(t+2)$ . We return to the pre-

vious analysis:

$$h(\mathbf{x}_{t+1}) \le h(\mathbf{y}_{t+1}) \le (1 - \mu_t) h(\mathbf{x}_t) + \mu_t^2 C$$

## Gap-based stepsize Choose $\gamma_t$ such that the term $-\gamma_t g(\mathbf{x}_t)$ +

 $\gamma_t^2 \frac{L}{2} \|\mathbf{s} - \mathbf{x}_t\|^2$  on the right-hand side of the inequality for  $h(\mathbf{x}_{t+1})$  a is minimized.

$$\gamma_t := \min\left(\frac{g(\mathbf{x}_t)}{L\|\mathbf{s} - \mathbf{x}_t\|^2}, 1\right)$$

## **Affinely Equivalent**

(f,X) and (f',X') are called affinely equivalent if  $f'(\mathbf{x}) = f(A\mathbf{x} + \mathbf{b})$  for some invertible matrix A and some vector **b**, and  $X' = \{A^{-1}(\mathbf{x} - \mathbf{b}) : \mathbf{x} \in X\}.$ 

We have  $\mathbf{x} \in X$  with function value  $f(\mathbf{x})$  if and only if  $\mathbf{x}' = A^{-1}(\mathbf{x} - \mathbf{b}) \in X'$  with the same function value  $f'(\mathbf{x}') = f(AA^{-1}(\mathbf{x} - \mathbf{b}) + \mathbf{b}) = f(\mathbf{x}).$ 

# Affine invariance of the Frank-Wolfe algorithm

The Frank-Wolfe algorithm is **invariant** under all affine transformations of space. Let (f, X) and (f', X') be affinely equivalent as befo-

The points **x** and  $\mathbf{x}' = \mathbf{A}^{-1}(\mathbf{x} - \mathbf{b}) \in X'$  are said to correspond to each other.

Chain rule:  $\nabla f'(\mathbf{x}') = \mathbf{A}^{\top} \nabla f(\mathbf{A}\mathbf{x}' + \mathbf{b}) = \mathbf{A}^{\top} \nabla f(\mathbf{x}).$ Now consider performing an iteration of the Frank-Wolfe algorithm

(a) on (f, X), starting from some iterate **x**, and (b) on (f', X'), starting from the corresponding itein both cases with the same stepsize.

Corresponding linear function values:

$$\nabla f'(\mathbf{x}')^{\top} \mathbf{z}' = \nabla f(\mathbf{x})^{\top} \mathbf{A} \mathbf{A}^{-1} (\mathbf{z} - \mathbf{b}) = \nabla f(\mathbf{x})^{\top} \mathbf{z} - c$$

where *c* some constant. Corresponding steps:  $\mathbf{s} = \text{LMO}_X(\nabla f(\mathbf{x}))$  if and only if  $\mathbf{s}' = \overline{\mathrm{LMO}_{X'}}(\nabla f'(\mathbf{x}'))$ 

$$C_{(f,X)} := \sup_{\substack{\mathbf{x},\mathbf{s} \in X, \gamma \in (0,1] \\ \mathbf{y} = (1-\gamma)\mathbf{x} + \gamma\mathbf{s}}} \frac{1}{\gamma^2} \Big( f(\mathbf{y}) - f(\mathbf{x}) - \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) \Big).$$
The curvature constant is affine invariant, i.e. if

(f,X) and (f',X') are affinely equivalent, then  $C_{(f,X)} = C_{(f',X')}$ . Thm 9.5 Convergence in terms of the curvature con-

# Consider the constrained minimization problem

where  $f: \mathbb{R}^d \to \mathbb{R}$  is convex, and set X is convex, closed and bounded. Let  $C_{(f,X)}$  be the curvature constant of f over X. With  $\mathbf{x}_0 \in X$ , and with stepsizes  $\gamma_t = 2/(t+2)$ , the Frank-Wolfe algorithm yields  $f(\mathbf{x}_T) - f(\mathbf{x}^*) \le \frac{4C_{(f,X)}}{T+1}, \quad T \ge 1$ 

$$\mathcal{O}(1/\varepsilon)$$
 many iterations are sufficent to obtain optimality gap at most  $\varepsilon$ .

**Lemma 9.6 Relating Curvature and Smoothness** Let f be a convex function which is smooth with

$$C_{(f,X)} \le \frac{L}{2} \operatorname{diam}(X)^2$$

# Convergence in duality gap

parameter L over X. Then

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be convex and smooth with parame- Assume  $R \ge 1/4$ . Then all iterates have value at least ter L, and  $\mathbf{x}_0 \in X, T \geq 2$ . Then choosing any of the three stepsizes that we have discussed, the Frank-Wolfe algorithm guarantees some t,  $1 \le t \le T$  such

$$g(\mathbf{x}_t) \le \frac{27/2 \cdot C_{(f,X)}}{T+1}, \quad T \ge 2$$

The smallest value  $g(\mathbf{x}_t)$ , t = 1,...,T bounds the optimality gap at iteration t:

$$f(\mathbf{x}_t) - f(\mathbf{x}^*) \le g(\mathbf{x}_t) \le \frac{27/2 \cdot C_{(f,X)}}{T+1}$$

This is a computable bound that certifies small optimality gap.

The current solution is a convex combination of  $\mathbf{x}_0$ and  $\mathcal{O}(1/\varepsilon)$  many extreme points (atoms) of the cons-Thinking of  $\varepsilon$  as a constant (such as 0.01): constantly many extreme points are sufficient in order to get

an almost optimal solution. Coreset: a small subsets of a given set of objects that is representative (with respect to some measure) for the set of all objects. Some algorithms for finding small coresets are vari-

ants of or inspired by the Frank-Wolfe algorithm

10. Newton's Method and Quasi-Newton Methods

**Newton-Raphson Method: 1-dim Case** Curvature constant (notion of complexity of (f, X)):

Method:

General update scheme: Goal: find a zero of differentiable  $f : \mathbb{R} \to \mathbb{R}$ .

 $\mathbf{q} \in \mathbb{R}^d$ .  $c \in R$ .

where  $\mathbf{H}(\mathbf{x}) \in \mathbb{R}^{d \times d}$  is some matrix.

Adaptive gradient descent

Newton's method:  $\mathbf{H} = \nabla^2 f(\mathbf{x}_t)^{-1}$ . Gradient descent:  $\mathbf{H} = \gamma \mathbf{I}$ . Newton's method: adaptive gradient descent, adap-

tation is w.r.t. the local geometry of the function at  $\mathbf{x}_t$ , as captured by the Hessian  $\nabla^2 f(\mathbf{x}_t)$ . Nondegenerate quadratic function A nondegenerate quadratic function is a function

of the form  $f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^{\top} \mathbf{M} \mathbf{x} - \mathbf{q}^{\top} \mathbf{x} + c$ 

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^{\mathsf{T}} \mathbf{M} \mathbf{x} - \mathbf{q}^{\mathsf{T}} \mathbf{x} + c$$

Let  $\mathbf{x}^* = \mathbf{M}^{-1} \mathbf{q}$  be the unique solution of  $\nabla f(\mathbf{x}) = \mathbf{0}$ .

 $\mathbf{x}^{\star}$  is the unique global minimum if f is convex.

Starting from  $x_0 > 0$ , we have  $x_{t+1} = \frac{1}{2} \left( x_t + \frac{R}{x_t} \right) \ge \frac{x_t}{2}.$ 

Newton-Raphson step:

Starting from 
$$x_0 = R \ge 1$$
, it takes at least  $\log(R)/2$ 

steps to get  $x_t < 2\sqrt{R}$ . But still only  $\mathcal{O}(\log R)$  steps to get  $x_t - \sqrt{R} < 1/2$ . (Proof see Hw10 Ex1)

 $x_{t+1} := x_t - \frac{f(x_t)}{f'(x_t)}, \quad t \ge 0.$ 

The Babylonian Method (Computing square roots)

Computing square roots: find a zero of  $f(x) = x^2$ 

 $x_{t+1} = x_t - \frac{f(x_t)}{f'(x_t)} = x_t - \frac{x_t^2 - R}{2x_t} = \frac{1}{2} \left( x_t + \frac{R}{x_t} \right).$ 

Suppose  $x_0 - \sqrt{R} < 1/2$  (achievable after  $\mathcal{O}(\log R)$ 

$$x_{t+1} - \sqrt{R} = \frac{1}{2} \left( x_t + \frac{R}{x_t} \right) - \sqrt{R} = \frac{1}{2x_t} \left( x_t - \sqrt{R} \right)^2$$

 $\sqrt{R} \ge 1/2$ . Hence we get

$$x_T - \sqrt{R} \le \left(x_0 - \sqrt{R}\right)^{2^T} < \left(\frac{1}{2}\right)^{2^T}, \quad T \ge 0.$$
To get  $x_T - \sqrt{R} < \varepsilon$ , we only need  $T = \log\log\left(\frac{1}{\varepsilon}\right)$ 

steps! **Newton's method for optimization** 

1-dimensional case

 $x_{t+1} - \sqrt{R} \le (x_t - \sqrt{R})^2$ 

#### Find a global minimum $x^*$ of a twice-differentiable convex function $f: \mathbb{R} \to \mathbb{R}$ .

Update step:

$$x_{t+1} := x_t - \frac{f'(x_t)}{f''(x_t)} = x_t - f''(x_t)^{-1} f'(x_t)$$

#### d-dimensional case Newton's method for minimizing a convex function

 $f: \mathbb{R}^d \to \mathbb{R}$ :

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \nabla^2 f(\mathbf{x}_t)^{-1} \, \nabla f(\mathbf{x}_t)$$

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^{\top} \mathbf{M} \mathbf{x} - \mathbf{q}^{\top} \mathbf{x} + c$$

 $\mathbf{x}_{t+1} = \mathbf{x}_t - \mathbf{H}(\mathbf{x}_t) \nabla f(\mathbf{x}_t),$ 

where 
$$\mathbf{M} \in \mathbb{R}^{d \times d}$$
 is an invertible symmetric matrix,

Lemma 10.1 Convergence in one step on quadratic On nondegenerate quadratic functions, with any starting point  $\mathbf{x}_0 \in \mathbb{R}^d$ , Newton's method yields

Lemma 10.3 Minimizing the second-order Taylor ap-Let f be convex and twice differentiable at  $\mathbf{x}_t \in$ dom(f), with  $\nabla^2 f(\mathbf{x}_t) > 0$  being invertible. The vec-

 $\mathbf{x}_{t+1} = \operatorname{argmin}$ 

tor  $\mathbf{x}_{t+1}$  resulting from the Netwon step satisfies

$$f(\mathbf{x}_t) + \nabla f(\mathbf{x}_t)^{\top} (\mathbf{x} - \mathbf{x}_t) + \frac{1}{2} (\mathbf{x} - \mathbf{x}_t)^{\top} \nabla^2 f(\mathbf{x}_t) (\mathbf{x} - \mathbf{x}_t)$$
  
Alternative interpretation of Newton's method: Each step minimizes the local second-order Taylor appro-

Thm 10.4 Convergence Thm Let  $f: dom(f) \to \mathbb{R}$  be twice differentiable with a critical point  $\mathbf{x}^*$ . Suppose there is a ball  $X \subseteq \text{dom}(f)$ with center  $x^*$ , s.t.

(i) Bounded inverse Hessians: There exists a real

$$\|\nabla^2 f(\mathbf{x})^{-1}\| \le \frac{1}{u}, \quad \forall \mathbf{x} \in X.$$

number u > 0 such that

(ii) Lipschitz continuous Hessians: There exists a real number B > 0 such that

$$\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\| \le B\|\mathbf{x} - \mathbf{y}\| \quad \forall \mathbf{x}, \mathbf{y} \in X.$$

Then, for  $\mathbf{x}_t \in X$  and  $\mathbf{x}_{t+1}$  resulting from the Newton step, we have

 $\|\mathbf{x}_{t+1} - \mathbf{x}^{\star}\| \le \frac{B}{2\mu} \|\mathbf{x}_t - \mathbf{x}^{\star}\|^2$ 

**Secant condition** Optimization for Data Science Yilei Tu, Page 10 of 14

#### Corollary 10.5 Super-exponentially fast With the assumptions and terminology of the con-

vergence theorem, and if

$$\left\|\mathbf{x}_0 - \mathbf{x}^{\star}\right\| \le \frac{\mu}{B}$$

then Newton's method yields

$$\|\mathbf{x}_T - \mathbf{x}^{\star}\| \le \frac{\mu}{B} \left(\frac{1}{2}\right)^{2^T - 1}, \quad T \ge 0$$

Starting close to the critical point, we will reach distance at most  $\varepsilon$  to it within  $\mathcal{O}(\log\log(1/\varepsilon))$  steps.

vergence theorem, and if  $\mathbf{x}_0 \in X$  satisfies

$$\|\mathbf{x}_0 - \mathbf{x}^{\star}\| \leq \frac{\mu}{B},$$

With the assumptions and terminology of the con-

Then the Hessians in Newton's method satisfy the relative error bound

$$\frac{\left\|\nabla^2 f(\mathbf{x}_t) - \nabla^2 f(\mathbf{x}^*)\right\|}{\left\|\nabla^2 f(\mathbf{x}^*)\right\|} \le \left(\frac{1}{2}\right)^{2^t - 1}, \quad t \ge 0.$$

# Lemma 10.7 Strong convexity ⇒ Bounded inverse

Let  $f: dom(f) \to \mathbb{R}$  be twice differentiable and strongly convex with parameter  $\mu$  over an open convex subset  $X \subseteq dom(f)$  meaning that

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^{\top} (\mathbf{y} - \mathbf{x}) + \frac{\mu}{2} ||\mathbf{x} - \mathbf{y}||^2, \quad \forall \mathbf{x}, \mathbf{y} \in X$$

Then  $\nabla^2 f(\mathbf{x})$  is invertible and  $\|\nabla^2 f(\mathbf{x})^{-1}\| \le 1/\mu$  for all  $\mathbf{x} \in X$ , where  $\|\cdot\|$  is the spectral norm.

# Secant Method: 1-dim Case

Use finite difference approximation of  $f'(x_t)$ :

$$f'(x_t) \approx \frac{f(x_t) - f(x_{t-1})}{x_t - x_{t-1}}.$$

(for  $|x_t - x_{t-1}|$  small) Obtain the secant method:

$$x_{t+1} := x_t - f(x_t) \frac{x_t - x_{t-1}}{f(x_t) - f(x_{t-1})}$$

Apply finite difference approximation to f'' (still

$$H_t := \frac{f'(x_t) - f'(x_{t-1})}{x_t - x_{t-1}} \approx f''(x_t)$$
$$f'(x_t) - f'(x_{t-1}) = H_t(x_t - x_{t-1})$$
the secant condition.

Newton's method:  $x_{t+1} := x_t - f''(x_t)^{-1} f'(x_t)$ 

secant condition

Secant method:  $x_{t+1} := x_t - H_t^{-1} f'(x_t)$ In higher dimensions: Let  $H_t \in \mathbb{R}^{d \times d}$  be an invertible symmetric matrix satisfying the *d*-dimensional

$$\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1}) = H_t(\mathbf{x}_t - \mathbf{x}_{t-1}).$$

The secant method step then becomes

$$\mathbf{x}_{t+1} := \mathbf{x}_t - H_t^{-1} \nabla f\left(\mathbf{x}_t\right).$$

# **Ouasi-Newton Methods**

condition

The secant method approximates Newton's method. • d = 1: unique number  $H_t$  satisfying the secant

• d > 1: Secant condition  $\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1}) =$  $H_t(\mathbf{x}_t - \mathbf{x}_{t-1})$  has infinitely many symmetric solutions  $H_t$  (underdetermined linear system).

Any scheme of choosing in each step of the secant method a symmetric  $H_t$  that satisfies the secant condition defines a Quasi Newton method. **Greenstadt's family of Quasi-Newton methods** 

Given: iterates  $\mathbf{x}_{t-1}$ ,  $\mathbf{x}_t$  as well as the matrix  $\mathbf{H}_{t-1}^{-1}$ . Wanted: next matrix  $\mathbf{H}_{t}^{-1}$  needed in next Quasi-Newton step

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \mathbf{H}_t^{-1} \, \nabla f \left( \mathbf{x}_t \right).$$

Greenstadt: Update

$$\mathbf{H}_t^{-1} := \mathbf{H}_{t-1}^{-1} + \mathbf{E}_t,$$

 $\mathbf{E}_t$  an error matrix. Try to minimize the error subject to  $\mathbf{H}_t$  satisfying the secant condition! Simple error measure: squared Frobenius norm

$$\|\mathbf{E}\|_F^2 := \sum_{i=1}^d \sum_{j=1}^d E_{ij}^2.$$

More general error measure

$$\|\mathbf{A}\mathbf{E}\mathbf{A}^{\top}\|_{F}^{2}$$
,

where  $\mathbf{A} \in \mathbb{R}^{d \times d}$  is some fixed invertible transformation matrix. A = I: squared Frobenius norm of E, the Specialized method.

The Greenstadt Update  $H_{t-1}^{-1} \rightarrow H_t^{-1}$ 

Secant condition in terms of  $H_t^{-1}$ :

$$H_t^{-1}\left(\nabla f\left(\mathbf{x}_t\right) - \nabla f\left(\mathbf{x}_{t-1}\right)\right) = \left(\mathbf{x}_t - \mathbf{x}_{t-1}\right).$$

Fix *t* and simplify notation:

$$\mathbf{H} := \mathbf{H}_{t-1}^{-1}$$

$$\mathbf{H}' := \mathbf{H}_t^{-1}$$
 (new inverse)  
 $\mathbf{E} := \mathbf{E}_t$ , (error matrix)

(old inverse)

$$\sigma := \mathbf{x}_t - \mathbf{x}_{t-1}$$
 (step in solutions)  
 $\mathbf{y} = \nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1})$  (step in gradients)

$$\mathbf{r} = \sigma - H\mathbf{y}$$
 (step in gradien

The update formula is

$$\mathbf{H}'=\mathbf{H}+\mathbf{E},$$

Secant condition becomes

$$\Leftrightarrow \mathbf{E}\mathbf{y} = \sigma - \mathbf{H}\mathbf{y} \quad \Leftrightarrow \quad \mathbf{E}\mathbf{y} = \mathbf{r}$$

 $\mathbf{H'}\mathbf{v} = \boldsymbol{\sigma} \Leftrightarrow (\mathbf{H} + \mathbf{E})\mathbf{v} = \boldsymbol{\sigma}$ 

Minimizing the error becomes a convex constrained minimization problem in the  $d^2$  variables  $E_{ij}$ :

minimize 
$$\frac{1}{2} \| \mathbf{A} \mathbf{E} \mathbf{A}^{\top} \|_{F}^{2}$$
 (error function) subject to  $\mathbf{E} \mathbf{y} = \mathbf{r}$  (secant condition)  $\mathbf{E}^{\top} = \mathbf{E}$  (symmetry)

Don't need to solve it computationally (for numbers  $E_{ij}$ ), but mathematically (formula for  $\mathbb{E}$ ). Minimize convex quadratic function subject to line-

ar equations → analytic formula for the minimizer from the method of Lagrange multipliers. Thm 10.8 (11.1) The method of Lagrange multipliers

Let  $f: \mathbb{R}^d \to \mathbb{R}$  be convex and differentiable,  $\mathbb{C} \in$ 

 $\mathbb{R}^{m \times d}$  for some  $m \in \mathbb{N}$ ,  $\mathbf{e} \in \mathbb{R}^m$ ,  $\mathbf{x}^{\star} \in \mathbb{R}^d$  such that  $Cx^* = e$ . Then the following two statements are equivalent.

(i) 
$$\mathbf{x}^* = \operatorname{argmin} \{ f(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^d, \mathbf{C}\mathbf{x} = \mathbf{e} \}$$

(ii) There exists a vector  $\lambda \in \mathbb{R}^m$  such that

$$\nabla f\left(\mathbf{x}^{\star}\right)^{\top} = \boldsymbol{\lambda}^{\top} \mathbf{C}$$

The entries of  $\lambda$  are known as the Lagrange multipliers.

Let  $\mathbf{M} \in \mathbb{R}^{d \times d}$  be a symmetric and invertible matrix. Consider the Quasi-Newton method

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \mathbf{H}_t^{-1} \, \nabla f(\mathbf{x}_t), \quad t \ge 1,$$

where  $\mathbf{H}_0 = \mathbf{I}$  (or any positive definite matrix), and  $\mathbf{H}_t^{-1} = \mathbf{H}_{t-1}^{-1} + \mathbf{E}_t$  for all  $t \ge 1$ . For any fixed t, set

$$\mathbf{E}^{\star} = \frac{1}{\mathbf{y}^{\top} \mathbf{M} \mathbf{y}} (\sigma \mathbf{y}^{\top} \mathbf{M} + \mathbf{M} \mathbf{y} \sigma^{\top} - \mathbf{H} \mathbf{y} \mathbf{y}^{\top} \mathbf{M} - \mathbf{M} \mathbf{y} \mathbf{y}^{\top} \mathbf{H}$$
$$-\frac{1}{\mathbf{y}^{\top} \mathbf{M} \mathbf{y}} (\mathbf{y}^{\top} \sigma - \mathbf{y}^{\top} \mathbf{H} \mathbf{y}) \mathbf{M} \mathbf{y} \mathbf{y}^{\top} \mathbf{M})$$

 $\mathbf{H} := \mathbf{H}_{t-1}^{-1}, \mathbf{H}' := \mathbf{H}_{t}^{-1}, \sigma := \mathbf{x}_{t} - \mathbf{x}_{t-1}, \mathbf{y} := \nabla f(\mathbf{x}_{t}) - \mathbf{y}_{t}$ 

If the update matrix  $\mathbf{E}_t = \mathbb{E}^*$  is used, the method is called the Greenstadt method with parameter M. Greenstadt suggested

$$\mathbf{M} = \mathbf{I}$$
 (default choice)  
 $\mathbf{M} = \mathbf{H}$  (previous inverse  $\mathbf{H}_{t-1}^{-1}$ )

#### **BFGS** method Chose M = H'. Secant condition holds: My = H'y =

Define

 $\sigma$ . M cancels. The BFGS method is the Greenstadt method with parameter  $\mathbf{M} := \mathbf{H}' = \mathbf{H}_t^{-1}$  in step t, in which case the update matrix  $E^*$  assumes the form

$$\mathbf{E}^{\star} = \frac{1}{\mathbf{y}^{\top} \sigma} \left( 2\sigma \sigma^{\top} - \mathbf{H} \mathbf{y} \sigma^{\top} - \sigma \mathbf{y}^{\top} \mathbf{H} - \frac{1}{\sigma^{\top} \mathbf{y}} \left( \mathbf{y}^{\top} \sigma - \mathbf{y}^{\top} \mathbf{H} \mathbf{y} \right) \sigma^{\top} \right)$$
$$= \frac{1}{\mathbf{y}^{\top} \sigma} \left( -\mathbf{H} \mathbf{y} \sigma^{\top} - \sigma \mathbf{y}^{\top} \mathbf{H} + \left( 1 + \frac{\mathbf{y}^{\top} \mathbf{H} \mathbf{y}}{\mathbf{y}^{\top} \sigma} \right) \sigma \sigma^{\top} \right)$$

where  $\mathbf{H} = \mathbf{H}_{t-1}^{-1}$ ,  $\sigma = \mathbf{x}_t - \mathbf{x}_{t-1}$ ,  $\mathbf{y} = \nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1})$ .

$$\mathbf{H}' = \mathbf{H} + \mathbf{E}^*$$

$$= \mathbf{H} + \frac{1}{\mathbf{v}^{\top} \sigma} \left\{ -\mathbf{H} \mathbf{y} \sigma^{\top} - \sigma \mathbf{y}^{\top} \mathbf{H} + \left( 1 + \frac{\mathbf{y}^{\top} \mathbf{H} \mathbf{y}}{\mathbf{v}^{\top} \sigma} \right) \sigma \sigma^{\top} \right\}$$

 $= \left(\mathbf{I} - \frac{\sigma \mathbf{y}^{\top}}{\mathbf{v}^{\top} \sigma}\right) \mathbf{H} \left(\mathbf{I} - \frac{\mathbf{y} \sigma^{\top}}{\mathbf{v}^{\top} \sigma}\right) + \frac{\sigma \sigma^{\top}}{\mathbf{v}^{\top} \sigma}$ 

Hw10 Ex4(i))

• 
$$\mathbf{y}^{\top} \sigma > 0$$
 unless  $\mathbf{x}_{t-1} = \mathbf{x}_t$  or  $f(\lambda \mathbf{x}_t + (1 - \lambda)\mathbf{x}_{t-1}) = \lambda f(\mathbf{x}_t) + (1 - \lambda)f(\mathbf{x}_{t-1})$  for all  $\lambda \in (0, 1)$ . (Proof see

- If  $\mathbf{y}^{\top} \boldsymbol{\sigma} > 0$  and **H** is positive definite, then also **H**? is positive definite. In this respect, the matrices in the BFGS method behave like proper inverse Hessians. (Proof see Hw10 Ex4(ii))
- Cost per update step:  $\mathcal{O}(d^2)$ , no Hessians and no inversions required.
- · Newton and Quasi-Newton methods are often performed with scaled steps. This means that the iteration becomes

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \alpha_t H_t^{-1} \nabla f(\mathbf{x}_t), \quad t \ge 1,$$

for some  $\alpha_t \in \mathbb{R}_+$ .

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# **Observation 10.9 (11.6)**

With  $E^*$  as in the BFGS method and  $H' = H + E^*$ , we have H'

1

**Lemma 10.10 (11.7) Efficiently computing matrix vector-products**  $\mathbf{H}_t^{-1} \nabla f(\mathbf{x}_t)$ Let  $\mathbf{H} = \mathbf{H}_{t-1}^{-1}$ ,  $\mathbf{H}' = \mathbf{H}_t^{-1}$  as in the BFGS method, i.e.

$$\mathbf{H'} = \left(\mathbf{I} - \frac{\sigma \mathbf{y}^{\top}}{\mathbf{v}^{\top} \sigma}\right) \mathbf{H} \left(\mathbf{I} - \frac{\mathbf{y} \sigma^{\top}}{\mathbf{v}^{\top} \sigma}\right) + \frac{\sigma \sigma^{\top}}{\mathbf{v}^{\top} \sigma}.$$

Let  $\mathbf{g}' \in \mathbb{R}^d$ . Suppose that we have an oracle to compute  $\mathbf{s} = \mathbf{H}\mathbf{g}$  for any vector  $\mathbf{g}$ . Then  $\mathbf{s}' = \mathbf{H}'\mathbf{g}'$  can be computed with one oracle call and  $\mathcal{O}(d)$  additional arithmetic operations, assuming that  $\sigma$  and  $\mathbf{y}$  are known.

The recursive BFGS-step (update step in one iterati-

In iteration t, call BFGS-STEP $(t, \nabla f(\mathbf{x}_t))$  to get

on) Handout10 Page 44

 $H_t^{-1} \nabla f(\mathbf{x}_t)$ .
Runtime  $\mathcal{O}(td)$ .

Worse than before if t > d.

The L-BFGS method (update step in one iteration) Handout10 Page 46

In iteration t, call L-BFGS-STEP(t, m,  $\nabla f$  ( $\mathbf{x}_t$ )) to get an approximation of  $\mathbf{H}_t^{-1} \nabla f$  ( $\mathbf{x}_t$ ) based on the previous m iterations.

Runtime per update  $\mathcal{O}(dm) = \mathcal{O}(d)$  if m is constant. 11. Modern Second-Order Methods and Nonconvex Optimization

#### Part A: Modern Second-order Methods Global analysis for strongly-convex smooth objecti-

ves • Assume  $f(\mathbf{x})$  is  $\mu$ -strongly convex and has L-

- Assume  $f(\mathbf{x})$  is  $\mu$ -strongly convex and has L Lipschitz continuous gradient.
- Consider Newton method  $\mathbf{x}_{t+1} := \mathbf{x}_t \gamma \nabla^2 f(\mathbf{x}_t)^{-1} \nabla f(\mathbf{x}_t)$ .
- We can show that Newton method enjoys a globally linear convergence with properly chosen stepsize  $\gamma>0$  :

$$f(\mathbf{x}_t) - f^* \le \left(1 - \frac{\mu^2}{L^2}\right)^t (f(\mathbf{x}_0) - f^*)$$

• Note that this is worse than GD, where

$$f\left(\mathbf{x}_{t}\right) - f^{*} \leq \left(1 - \frac{\mu}{L}\right)^{t} \left(f\left(\mathbf{x}_{0}\right) - f^{*}\right)$$

### Overcoming the local nature of Newton method

• Newton method with line-search: select  $\gamma_t$  such that  $f(\mathbf{x}_{t+1}) < f(\mathbf{x}_t)$  with sufficient decrease.

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \nabla^2 f(\mathbf{x}_t)^{-1} \nabla f(\mathbf{x}_t)$$

• Damped Newton method:

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \frac{1}{1 + \lambda_f(\mathbf{x}_t)} \nabla^2 f(\mathbf{x}_t)^{-1} \nabla f(\mathbf{x}_t),$$

where  $\lambda_f(\mathbf{x}) = \left\| \left[ \nabla^2 f(\mathbf{x}) \right]^{-1/2} \nabla f(\mathbf{x}) \right\|$  is the Newton decrement.

• Regularization approach: regularize the Hessian and adjust  $\gamma_t$  properly

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \left[ \gamma_t I + \nabla^2 f(\mathbf{x}_t) \right]^{-1} \nabla f(\mathbf{x}_t)$$

• Trust-region approach:

$$\mathbf{x}_{t+1} = \underset{\mathbf{x}}{\operatorname{argmin}} \quad f(\mathbf{x}_t) + \nabla f(\mathbf{x}_t)^{\top} (\mathbf{x} - \mathbf{x}_t)$$
$$+ \frac{1}{2} (\mathbf{x} - \mathbf{x}_t)^{\top} \nabla^2 f(\mathbf{x}_t) (\mathbf{x} - \mathbf{x}_t)$$
$$\text{s.t. } ||\mathbf{x} - \mathbf{x}_t|| \leq \Delta_k.$$

#### **Lipschitz Hessian**

• Recall for functions f with  $L_1$ -Lipschitz gradient, we have

$$f(\mathbf{x}) \le f(\mathbf{x}_t) + \nabla f(\mathbf{x}_t)^{\top} (\mathbf{x} - \mathbf{x}_t) + \frac{L_1}{2} ||\mathbf{x} - \mathbf{x}_t||^2$$

GD can be viewed as iteratively minimizing the quadratic upper bound function.

• Now assuming f has  $L_2$ -Lipschitz Hessian, similarly, we can show that

$$f(\mathbf{x}) \le f(\mathbf{x}_t) + \nabla f(\mathbf{x}_t)^{\top} (\mathbf{x} - \mathbf{x}_t)$$
  
+ 
$$\frac{1}{2} (\mathbf{x} - \mathbf{x}_t)^{\top} \nabla^2 f(\mathbf{x}_t) (\mathbf{x} - \mathbf{x}_t) + \frac{L_2}{6} ||\mathbf{x} - \mathbf{x}_t||^3$$

(Proof see Hw11 Ex4)

**Cubic Regularization: The Algorithm** 

$$\begin{aligned} \mathbf{x}_{t+1} &\in \underset{\mathbf{x}}{\operatorname{argmin}} \hat{f}\left(\mathbf{x}, \mathbf{x}_{t}\right) \\ \hat{f}\left(\mathbf{x}, \mathbf{x}_{t}\right) &:= f\left(\mathbf{x}_{t}\right) + \nabla f\left(\mathbf{x}_{t}\right)^{\top} \left(\mathbf{x} - \mathbf{x}_{t}\right) \\ &+ \frac{1}{2} \left(\mathbf{x} - \mathbf{x}_{t}\right)^{\top} \nabla^{2} f\left(\mathbf{x}_{t}\right) \left(\mathbf{x} - \mathbf{x}_{t}\right) + \frac{M}{6} \left\|\mathbf{x} - \mathbf{x}_{t}\right\|^{3} \end{aligned}$$

**Cubic Regularization: Global Analysis Key facts:** 

•  $\nabla^2 f(\mathbf{x}_t) + \frac{M}{2} ||\mathbf{x}_t - \mathbf{x}_{t+1}|| \cdot I \ge 0$ •  $||\nabla f(\mathbf{x}_{t+1})|| \le \frac{L_2 + M}{2} ||\mathbf{x}_t - \mathbf{x}_{t+1}||^2$ 

•  $-f(\mathbf{x}_t) - f(\mathbf{x}_{t+1}) \ge \frac{M}{12} ||\mathbf{x}_t - \mathbf{x}_{t+1}||^3 \text{ if } M \ge L_2.$ 

Implications

• Convergence to a second-order stationary point: If  $\mathbf{x}^*$  is a limiting point, then  $\nabla f(\mathbf{x}^*) = 0, \nabla^2 f(\mathbf{x}^*) \geq 0$ 

- Convergence rate: We have  $\min_{1 \le i \le t} \|\nabla f(\mathbf{x}_i)\| = \mathcal{O}\left(\frac{1}{t^{2/3}}\right)$ .
- Convex setting: If f is convex, we have  $f(\mathbf{x}_t) f^* = \mathcal{O}\left(\frac{1}{t^2}\right)$ .
- Strongly convex setting: If *f* is strongly convex, it implies superlinear convergence.

(Proof see Handout11 Page 14)

Cubic Regularization: Extension

- Accelerated Cubic Regularization: For convex functions, can achieve  $\mathcal{O}\left(\frac{1}{t^3}\right)$  convergence rate
- High-order Tensor Method: For convex functions and p-th order method, can achieve  $\mathcal{O}\left(\frac{1}{t^{p+1}}\right)$  convergence rate.
- Lower bound: For *p*-th order method, the lower complexity bound is  $\Omega\left(\frac{1}{t^{(3p+1)/2}}\right)$

# Part B: Modern Nonconvex Optimization

Consider the stochastic optimization problem:

$$\min_{\mathbf{x} \in \mathbb{R}^d} F(\mathbf{x}) := \mathbb{E}_{\boldsymbol{\xi}}[f(\mathbf{x}, \boldsymbol{\xi})] \quad \left[ \text{ or } F(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x}) \right]$$

SGD:

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \gamma_t \nabla f(\mathbf{x}_t, \boldsymbol{\xi}_t)$$
, where  $\boldsymbol{\xi}_t \stackrel{iid}{\sim} P(\boldsymbol{\xi})$ 

# Thm 11.1 Convergence of Nonconvex SGD Assume that

• Function *F* is *L*-smooth,

• The unbiased estimator satisfies that for all  $\mathbf{x}$ :  $\mathbb{E}\left[\|\nabla f(\mathbf{x}, \boldsymbol{\xi}) - \nabla F(\mathbf{x})\|_2^2\right] \le \sigma^2$ .

Under the above assumption, SGD with  $\gamma_t = \min\left\{\frac{1}{L}, \frac{\gamma}{\sigma\sqrt{T}}\right\}$  achieves:

$$\mathbb{E}\left[\left\|\nabla F\left(\hat{\mathbf{x}}_{T}\right)\right\|^{2}\right] \leq \frac{\sigma}{\sqrt{T}}\left(\frac{2\left(F\left(\mathbf{x}_{1}\right) - F\left(\mathbf{x}^{*}\right)\right)}{\gamma} + L\gamma\right)$$

where  $\hat{\mathbf{x}}_T$  is selected uniformly at random from  $\{\mathbf{x}_1, \dots, \mathbf{x}_T\}$ .

Handout11 Pages 29-30
Stationary Points
A stationary point can be a local minimum, a local

Variance-reduced SGD for Nonconvex Optimization

A stationary point can be a local minimum, a local maximum, or a saddle point.

- If  $\nabla^2 F(\overline{\mathbf{x}}) > 0$ , then  $\overline{\mathbf{x}}$  is a local minimum.
- If  $\nabla^2 F(\overline{\mathbf{x}}) < 0$ , then  $\overline{\mathbf{x}}$  is a local maximum.
- If  $\nabla^2 F(\overline{\mathbf{x}})$  has positive and negative eigenvalues, then  $\overline{\mathbf{x}}$  is a (strict) saddle point.
- Otherwise, it remains inconclusive.

Thm 11.2 GD with Random Initialization (informal) If f satisfies the strict saddle property, then GD with random initialization and sufficiently small

constant stepsize converges to a local minimum or

negative infinity almost surely. The analysis is not specific to GD and can apply to other algorithms. \*Noisy SGD

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta \nabla f\left(\mathbf{x}_t, \xi_t\right) + \mathbf{z}$$

where the noise  $\mathbf{z}$  is uniformly sampled from unit sphere.

# Thm 11.3 (informal)

If f satisfies the strict saddle property and has Lipschitz Hessian, then Noisy SGD with sufficiently small stepsize converges to an  $\epsilon$ -second order stationary point in  $\operatorname{poly}(d/\epsilon)$  steps. Handout11 Page 41

Convergence to global minima

For problems with benign nonconvexity. Handout11 Page 44

**12. Modern Nonsmooth Optimization** Part A: Mirror Descent

Bregman Divergence

Let  $\omega(\cdot): \Omega \to \mathbb{R}$  be continuously differentiable on  $\Omega$  and 1-strongly convex w.r.t. some norm  $\|\cdot\|: \omega(\mathbf{x}) \ge \omega(\mathbf{y}) + \nabla \omega(\mathbf{y})^\top (\mathbf{x} - \mathbf{y}) + \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|^2, \forall x, y \in \Omega$ .

The Bregman divergence is defined as

$$V_{\omega}(\mathbf{x}, \mathbf{y}) = \omega(\mathbf{x}) - \omega(\mathbf{y}) - \nabla \omega(\mathbf{y})^{\top} (\mathbf{x} - \mathbf{y}), \forall \mathbf{x}, \mathbf{y} \in \Omega$$

which implies

$$V_{\omega}(\mathbf{x}, \mathbf{y}) \ge \frac{1}{2} ||\mathbf{x} - \mathbf{y}||^2$$

### xamples

• Euclidean distance:  $\Omega = \mathbb{R}^d$ ,  $\omega(\mathbf{x}) = \frac{1}{2} ||\mathbf{x}||_2^2$ ,  $||\cdot|| = ||\cdot||_2$ 

$$V_{\omega}(\mathbf{x}, \mathbf{y}) = \frac{1}{2} ||\mathbf{x} - \mathbf{y}||_2^2$$

• Mahalanobis distance:  $\Omega = \mathbb{R}^d$ ,  $\omega(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{Q}\mathbf{x}$  (where  $\mathbf{Q} \ge \mathbf{I}$ ),  $\|\cdot\| = \|\cdot\|_2$ ,

$$V_{\omega}(\mathbf{x}, \mathbf{y}) = \frac{1}{2}(\mathbf{x} - \mathbf{y})^{\top} \mathbf{Q}(\mathbf{x} - \mathbf{y})$$

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**Examples**
• Subgradient descent: 
$$\omega(\mathbf{x}) = \frac{1}{2} ||\mathbf{x}||_2^2$$
,  $V_{\omega}(\mathbf{x}, \mathbf{x}_t) =$ 

 $\frac{1}{2} \|\mathbf{x} - \mathbf{x}_t\|_2^2$ Kullback-Leibler divergence:  $\Omega = \Delta_d, \omega(\mathbf{x}) =$ 

$$\sum_{i=1}^{d} x_i \log x_i, \|\cdot\| = \|\cdot\|_1,$$

$$V_{\omega}(\mathbf{x}, \mathbf{y}) = \mathrm{KL}(\mathbf{x} \mid \mathbf{y}) := \sum_{i=1}^{u} x_i \log \frac{x_i}{y_i}$$

# **Properties** • Nonnegativity: $V_{(i)}(\mathbf{x}, \mathbf{y}) \geq 0$ .

- Convexity:  $V_{\alpha}(\mathbf{x}, \mathbf{y})$  is convex in  $\mathbf{x}$ . •  $V_{(i)}(\mathbf{x}, \mathbf{y}) \ge \frac{1}{2} ||\mathbf{x} - \mathbf{y}||^2$ .
- Non-symmetry:  $V_{\omega}(\mathbf{x}, \mathbf{y}) \neq V_{\omega}(\mathbf{y}, \mathbf{x})$  in general.
- Generalized Pythagorean Theorem: Define the Bregman projection of a point **z** onto *X* as:
- $\Pi_X^{\omega}(\mathbf{z}) := \underset{\mathbf{x} \in X}{\operatorname{argmin}} V_{\omega}(\mathbf{x}, \mathbf{z}).$

Then for any 
$$x \in X, z \in \Omega$$
 it holds that

 $V_{\omega}(\mathbf{x}, \mathbf{z}) \ge V_{\omega}(\mathbf{x}, \Pi_{X}^{\omega}(\mathbf{z})) + V_{\omega}(\Pi_{X}^{\omega}(\mathbf{z}), \mathbf{z})$ 

# Lemma 12.1 Three Point Identity

the optimality condition,

$$\begin{aligned} V_{\omega}(\mathbf{x}, \mathbf{z}) = & V_{\omega}(\mathbf{x}, \mathbf{y}) + V_{\omega}(\mathbf{y}, \mathbf{z}) - \langle \nabla \omega(\mathbf{z}) - \nabla \omega(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle \\ & \forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \Omega \end{aligned}$$

**Special case:**  $\omega(\mathbf{x}) = \frac{1}{2} ||\mathbf{x}||_2^2$ , this is the **law of cosine**:

$$\|\mathbf{x} - \mathbf{z}\|_{2}^{2} = \|\mathbf{x} - \mathbf{y}\|_{2}^{2} + \|\mathbf{y} - \mathbf{z}\|_{2}^{2} - 2\langle \mathbf{z} - \mathbf{y}, \mathbf{x} - \mathbf{y} \rangle$$

# Corollary of Lemma 12.1 Three Point Identity Since $\mathbf{x}_{t+1} = \operatorname{argmin}_{\mathbf{x} \in X} \{ V_{\omega}(\mathbf{x}, \mathbf{x}_t) + \langle \gamma_t \mathbf{g}_t, \mathbf{x} \rangle \}$ , by

 $\langle \nabla \omega (\mathbf{x}_{t+1}) + \gamma_t \mathbf{g}_t - \nabla \omega (\mathbf{x}_t), \mathbf{x} - \mathbf{x}_{t+1} \rangle \geq 0, \forall \mathbf{x} \in X$ 

$$\Rightarrow \langle \nabla \omega (\mathbf{x}_{t+1}) - \nabla \omega (\mathbf{x}_t), \mathbf{x} - \mathbf{x}_{t+1} \rangle \ge \langle \gamma_{tt}, \mathbf{x}_{t+1} - \mathbf{x} \rangle$$

From three point identity, we have for 
$$\forall \mathbf{x} \in X$$
:

 $\langle \gamma_t \mathbf{g}_t, \mathbf{x}_{t+1} - \mathbf{x} \rangle \le \langle \nabla (\mathbf{x}_{t+1}) - \nabla \omega (\mathbf{x}_t), \mathbf{x} - \mathbf{x}_{t+1} \rangle$  $= V_{\omega}(\mathbf{x}, \mathbf{x}_{t}) - V_{\omega}(\mathbf{x}, \mathbf{x}_{t+1}) - V_{\omega}(\mathbf{x}_{t+1}, \mathbf{x}_{t})$ 

$$|\mathbf{x}_{t+1}| - \underbrace{V_{\omega}(\mathbf{x}_{t+1}, \mathbf{x}_t)}_{\geq \frac{1}{2} ||\mathbf{x}_t - \mathbf{x}_{t+1}||^2}$$
 satisfies that

# **Mirror Descent Algorithm**

$$\mathbf{x}_{t+1} = \underset{\mathbf{x} \in X}{\operatorname{argmin}} \{ V_{\omega}(\mathbf{x}, \mathbf{x}_t) + \langle \gamma_t \mathbf{g}_t, \mathbf{x} \rangle \}, \text{ where } \mathbf{g}_t \in \partial f(\mathbf{x}_t)$$
 Subgradient descent:

**Examples** 

$$\mathbf{x}_{t+1} = \Pi_X \left( \mathbf{x}_t - \gamma_t \mathbf{g}_t \right)$$

 $\sum_{i=1}^{d} x_i \log x_i, V_{(i)}(\mathbf{x}, \mathbf{x}_t) = \mathrm{KL}(\mathbf{x} \mid \mathbf{x}_t).$  $\mathbf{x}_{t+1} \propto \mathbf{x}_t \odot \exp(-\gamma_t \mathbf{g}_t)$ 

Let f be convex and  $\omega(\cdot)$  be 1-strongly convex on X w.r.t. norm  $\|\cdot\|$ .

$$\gamma_{t}\left(f\left(\mathbf{x}_{t}\right)-f^{*}\right)\leq V_{\omega}\left(\mathbf{x}^{*},\mathbf{x}_{t}\right)-V_{\omega}\left(\mathbf{x}^{*},\mathbf{x}_{t+1}\right)+\frac{\gamma_{t}^{2}}{2}\left\|\mathbf{g}_{t}\right\|_{*}^{2}$$

# Theorem 12.3

Suppose f is B-Lipschitz continuous such that  $|f(\mathbf{x})|$  $|f(\mathbf{y})| \leq B||\mathbf{x} - \mathbf{y}||$ , namely,  $||\mathbf{g}||_* \leq B$  for any  $\mathbf{g} \in \partial f(\mathbf{x})$ . Define  $R^2 := \sup_{\mathbf{x} \in X} V_{(t)}(\mathbf{x}, \mathbf{x}_1)$ , where  $R \ge 0$  and set

 $\min_{1 \le t \le T} f(\mathbf{x}_t) - f^* \le \frac{V_{\omega}(\mathbf{x}^*, \mathbf{x}_1) + \frac{1}{2} \sum_{t=1}^{T} \gamma_t^2 \|\mathbf{g}_t\|_*^2}{\sum_{t=1}^{T} \gamma_t}$ 

# **Mirror Descent for Smooth Objectives**

Consider the problem  $\min_X f(\mathbf{x})$ , where X is closed and convex, and f is convex and L-smooth such that  $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_* \le L \|\mathbf{x} - \mathbf{y}\|_* \ \forall \mathbf{x}, \mathbf{y} \in X$  for some norm || · ||. This further implies that

 $\min_{1 \le t \le T} f(\mathbf{x}_t) - f^* \le \mathcal{O}\left(\frac{BR}{\sqrt{T}}\right).$ 

$$f(\mathbf{x}) \le f(\mathbf{y}) + \langle \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle + \frac{L}{2} ||\mathbf{x} - \mathbf{y}||^2.$$

By setting  $\gamma_t = 1/L$ , the sequence of iterates  $\{ \curvearrowright_t \}$ generated by Mirror Descent:

$$\mathbf{x}_{t+1} = \underset{\mathbf{x} \in X}{\operatorname{argmin}} \left\{ V_{\omega} \left( \mathbf{x}, \mathbf{x}_{t} \right) + \left\langle \gamma_{t} \nabla f \left( \mathbf{x}_{t} \right), \mathbf{x} \right\rangle \right\}$$

$$\min_{1 \le t \le T} f(\mathbf{x}_{t+1}) - f(\mathbf{x}^*) \le \frac{L \cdot V_{\omega}(\mathbf{x}^*, \mathbf{x}_1)}{T}$$

Subgradient descent: special case with  $\|\cdot\| = \|\cdot\|_2$ and  $\omega(\cdot) = \frac{1}{2} || \cdot ||_2^2$ .

**Optimization over simplex** Assume  $\|\mathbf{g}\|_{\infty} \leq 1, \forall \mathbf{g} \in \partial f(\mathbf{x})$  and  $X = \Delta_d$ . Set  $\mathbf{x}_1 = [1/d; ...; 1/d].$ 

**Conjugate Function** 

- Subgradient Descent:  $\mathcal{O}\left(\frac{\sqrt{d}}{\sqrt{T}}\right)$ , where B = $\mathcal{O}(\sqrt{d}), R = \mathcal{O}(1).$
- Entropic descent:  $X = \Delta_d$ ,  $\omega(\mathbf{x}) = \bullet$  Mirror Descent:  $\mathcal{O}\left(\frac{\sqrt{\log d}}{\sqrt{T}}\right)$ , where  $B = \mathcal{O}(1), R = \frac{1}{2}$  $\mathcal{O}(\sqrt{\log d})$ .

Part B: Smoothing Techniques **Convex Conjugate Theory** 

 $f^{\star}(\mathbf{y}) = \sup_{\mathbf{x} \in \text{dom}(f)} \{\mathbf{y}^T \mathbf{x} - f(\mathbf{x})\}$ 

The conjugate function of f is

Fenchel's inequality 
$$f(\mathbf{x}) + f^*(\mathbf{y}) \ge \mathbf{x}^T \mathbf{y}, \forall \mathbf{x}, \mathbf{y}$$
  
Lemma 12.5  
(1) Duality: If  $f$  is lower semi-continuous (l.s.c.)

also called Legendre-Fenchel transformation.

and convex, then  $f^{**} = f$ . Function f is l.s.c. if  $f(\mathbf{x}) \leq \liminf_{t \to \infty} f(\mathbf{x}_t)$  for (2) Fenchel's inequality:  $\mathbf{x}^T \mathbf{y} \leq f(\mathbf{x}) + f^*(\mathbf{y})$ .

- (3) If f and g are l.s.c. and convex, then  $(f+g)^*(\mathbf{x}) =$  $\inf_{\mathbf{v}} \{ f^{\star}(\mathbf{y}) + g^{\star}(\mathbf{x} - \mathbf{y}) \}.$
- (4) If f is  $\mu$ -strongly convex, then  $f^*$  is differentiable and  $\frac{1}{u}$ -smooth.

- Quadratic:  $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{Q}\mathbf{x}$  where  $\mathbf{Q} > 0$ ,  $f^*(y) =$  $\frac{1}{2}\mathbf{v}^T\mathbf{O}^{-1}\mathbf{v}$ • Negative entropy:  $f(\mathbf{x}) = \sum_{i=1}^{n} x_i \log(x_i), f^*(\mathbf{y}) =$
- Negative logarithm:  $f(\mathbf{x}) = -\sum_{i=1}^{n} \log(x_i), f^*(\mathbf{y}) =$
- Norm:  $f(\mathbf{x}) = ||\mathbf{x}||, f^*(\mathbf{y}) = \begin{cases} 0, & ||\mathbf{y}||_* \le 1 \\ +\infty, & ||\mathbf{y}||_* > 1 \end{cases}$

**Part B: Smoothing Techniques Nesterov's Smoothing for Convex Functions** Assume f is convex, then  $f(\mathbf{x}) = (f^*)^* =$ 

 $-\sum_{i=1}^{n}\log(-y_i)-n$ .

 $\max_{\mathbf{y}} \{ \mathbf{x} \mid \mathbf{y} - f^*(\mathbf{y}) - \mu \cdot d(\mathbf{y}) \}.$ **Nesterov's Smoothing is** 

 $f_{\mu}(\mathbf{x}) = \max_{\mathbf{y} \in \text{dom}(f^{*})} \left\{ \mathbf{x}^{T} \mathbf{y} - f^{*}(\mathbf{y}) - \mu \cdot d(\mathbf{y}) \right\} = \left( f^{*} + \mu d(\cdot) \right)^{*}$ 

$$\mathbf{x}) = \max_{\mathbf{y} \in \text{dom}(f^*)} \left\{ \mathbf{x}^T \mathbf{y} - f^*(\mathbf{y}) - \mu \cdot d(\mathbf{y}) \right\} = \left( f^* + \mu d(\cdot) \right)$$

• Here  $f^*(y)$  is the convex conjugate of f.

 $-d(\mathbf{y}) = \frac{1}{2} ||\mathbf{y} - \mathbf{y}_0||_2^2$  $-d(\mathbf{y}) = \frac{1}{2} \sum w_i (y_i - y_{0,i})^2$  with  $w_i \ge 1$ ;

• Proximity function: d(y) is 1-strongly convex and

-  $d(\mathbf{y}) = \omega(\mathbf{y}) - \omega(\mathbf{y}_0) - \nabla \omega(\mathbf{y}_0)^{\top} (\mathbf{y} - \mathbf{y}_0)$  with  $\omega(\mathbf{x})$  being 1-strongly convex.

nonnegative everywhere.

- Smoothness: Function  $f_{\mu}(\mathbf{x})$  is  $\frac{1}{\mu}$ -smooth. • Approximation: For convex f with bounded
- $dom(f^*)$ , we have

 $f(\mathbf{x}) - f^* \le f(\mathbf{x}) - f_{\mu}(\mathbf{x}) + f_{\mu}(\mathbf{x}) - \min_{\mathbf{x}} f_{\mu}(\mathbf{x})$ 

 $f(\mathbf{x}) - \mu D^2 \le f_{\mu}(\mathbf{x}) \le f(\mathbf{x})$ , where  $D^2 = \max_{\mathbf{y} \in \text{dom}(f^*)} d(\mathbf{y})$ 

approximation error optimization error • If we apply Accelerated Gradient Descent to solve the smoothed problem:

$$f(\mathbf{x}_t) - f^* \le \mathcal{O}\left(\mu D^2 + \frac{R^2}{\mu t^2}\right) \le \epsilon$$
 To achieve accuracy  $\epsilon > 0$ , need  $\mu = \mathcal{O}\left(\frac{\epsilon}{D^2}\right)$ .

The number of AGD iterations is at most  $T_{\epsilon}$  =

 $\mathcal{O}\left(\frac{R}{\sqrt{\epsilon u}}\right) = \mathcal{O}\left(\frac{RD}{\epsilon}\right)$ **Moreau-Yosida Regularization for Convex Functions** 

$$f_{\mu}(\mathbf{x}) = \min_{\mathbf{y}} \left\{ f(\mathbf{y}) + \frac{1}{2\mu} ||\mathbf{x} - \mathbf{y}||_{2}^{2} \right\}$$

- Here  $\mu > 0$  and  $f_{\mu}(\mathbf{x})$  is called the Moreau envelope of  $f(\mathbf{x})$ .
- Huber function is Moreau envelope of f(x) = |x|:

$$f_{\mu}(x) = \begin{cases} \frac{x^2}{2\mu}, & |x| \le \mu \\ |x| - \frac{\mu}{2}, & |x| > \mu \end{cases}$$

• M-Y Regularization is a special case of Nesterov's smoothing with  $d(\mathbf{y}) = \frac{1}{2} ||\mathbf{y}||^2$ .

$$f_{\mu}(\mathbf{x}) = \max_{\mathbf{y}} \left\{ \mathbf{x}^{T} \mathbf{y} - f^{\star}(\mathbf{y}) - \frac{\mu}{2} ||\mathbf{y}||_{2}^{2} \right\}$$
$$= \left( f^{\star} + \frac{\mu}{2} || \cdot ||_{2}^{2} \right)^{\star} (\mathbf{x})$$
$$= \inf_{\mathbf{y}} \left\{ f(\mathbf{y}) + \frac{1}{2\mu} ||\mathbf{x} - \mathbf{y}||_{2}^{2} \right\}$$

#### Optimization for Data Science Yilei Tu, Page 13 of 14 PPA: $\mathbf{x}_{t+1} = \operatorname{prox}_{\lambda_t f} (\mathbf{x}_t)$ • Smoothness: Function $f_{\mu}(\mathbf{x})$ is $\frac{1}{\mu}$ -smooth.

- Exact Minimization:  $\min_{\mathbf{x}} f(\mathbf{x}) = \min_{\mathbf{x}} f_{\mu}(\mathbf{x})$ .
- $\operatorname{prox}_{\mu f}(\mathbf{x}) := \operatorname{argmin}_{\mathbf{y}} \left\{ f(\mathbf{y}) + \frac{1}{2\mu} \|\mathbf{x} \mathbf{y}\|_{2}^{2} \right\}$

 $\nabla f_{\mu}(\mathbf{x}) = \frac{1}{u} \left( \mathbf{x} - \operatorname{prox}_{\mu f}(\mathbf{x}) \right)$ GD on smooth  $f_{\mu}(\mathbf{x})$  reduces to proximal minimi-

zation on 
$$f(\mathbf{x})$$
:  

$$\mathbf{x}_{t+1} = \mathbf{x}_t - \mu \nabla f_u(\mathbf{x}_t) \Longleftrightarrow \mathbf{x}_{t+1} = \operatorname{prox}_{uf}(\mathbf{x}_t)$$

#### The proximal operator of convex function g at $\mathbf{x}$ is defined as

$$\operatorname{prox}_{f}(\mathbf{x}) = \underset{\mathbf{y}}{\operatorname{argmin}} \left\{ f(\mathbf{y}) + \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_{2}^{2} \right\}$$

For continuous convex function f,  $prox_f(\mathbf{x})$  exists For many nonsmooth functions, proximal operators

can be computed efficiently (closed form solution, low-cost computation, polynomial time).

# **Properties**

- Let g be a convex function with  $dom(g) = \mathbb{R}^d$ . Then
- (Subgradient characterization) y = prox<sub>σ</sub>(x) ⇐⇒  $\mathbf{x} - \mathbf{y} \in \partial g(\mathbf{y}).$
- (Fixed Point) A point  $x^*$  minimizes  $g(x) \iff x^* =$
- $\|{\bf x} {\bf y}\|_2$ . (Proof see Hw12 Ex3)

• (Non-expansiveness)  $\left\| \operatorname{prox}_{g}(\mathbf{x}) - \operatorname{prox}_{g}(\mathbf{y}) \right\|_{2} \leq$ 

- If  $f(\mathbf{x}) = \delta_X(\mathbf{x}) = \begin{cases} 0, & \mathbf{x} \in X \\ +\infty, & \mathbf{x} \notin X \end{cases}$ , then  $\operatorname{prox}_f(\mathbf{x}) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\mathbf{x} \cdot \mathbf{x}}{\mathbf{x} \cdot \mathbf{x}} d\mathbf{x}$  $\Pi_X(\mathbf{x})$  is the projection.
- If  $f(\mathbf{x}) = \mu ||\mathbf{x}||_1$ , then  $\operatorname{prox}_f(\mathbf{x})$  is the soft thresholding operator.
- $\operatorname{prox}_{\mu|\cdot|}(x_i) = \begin{cases} x_i \mu & \text{if } x_i > \mu \\ 0 & \text{if } |x_i| \le \mu \\ x_i + \mu & \text{if } x_i < -\mu \end{cases}$

Equivalently,  $\operatorname{prox}_{\mu||.||_1}(\mathbf{x}) = \operatorname{sign}(\mathbf{x}) \odot \max\{|\mathbf{x}| - \mu, 0\}$ 

# **Proximal Point Algorithm**

**Theorem 12.7 Convergence of PPA** If f is convex, then for any  $T \ge 1$ ,

 $f(\mathbf{x}_{T+1}) - f^* \le \frac{\|\mathbf{x}_1 - \mathbf{x}^*\|_2^2}{2\sum_{t=1}^T \lambda_t}.$ 

**Smoothing Techniques for Nonconvex Functions Lasry-Lions Regularization** 

Setting  $\lambda_t = \lambda$ , this implies a  $\mathcal{O}(1/t)$  convergence

Handout12 Page 43 **Randomized Smoothing** Handout12 Page 44 13. Min-Max Optimization

13.1 Min-Max Optimization **Min-Max Optimization** Let  $\mathcal{X} \subset \mathbb{R}^d$ ,  $\mathcal{Y} \subset \mathbb{R}^p$  and  $\phi : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ . Consider the min-max problem:

 $\min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \phi(\mathbf{x}, \mathbf{y})$ **Zero-sum Matrix Games Max-Min Inequality** 2-players games where players have opposite eva-

#### luations of outcomes: • I (resp. I ) non-empty finite set of strategies of player 1 (resp. player 2).

• payoff of player 1 given by a real-valued  $I \times I$  matrix A (resp. -A for player 2).• Set of mixed strategies

 $\{\mathbf{x} \in \mathbb{R}^{|I|} : \mathbf{x}_i \ge 0, i \in I, \sum_{i \in I} \mathbf{x}_i = 1\}$  of player 1 (resp.  $\Delta(J)$  for player 2).

 $\min \max_{\mathbf{x}} \mathbf{x}^T \mathbf{A} \mathbf{y}$ 

# **Nonsmooth Optimization**

matrix and consider the problem:

$$\min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) + g(\mathbf{A}\mathbf{x})$$

Recall that  $g(\mathbf{A}\mathbf{x}) = \max_{\mathbf{y} \in \mathbb{R}^p} \langle \mathbf{A}\mathbf{x}, \mathbf{y} \rangle - g^*(\mathbf{y})$  where  $g^*$ is the Fenchel conjugate. Then the problem is equivalent to Min-Max refor-

$$\min_{\mathbf{x} \in \mathbb{R}^d} \max_{\mathbf{y} \in \mathbb{R}^p} f(\mathbf{x}) + \langle \mathbf{A}\mathbf{x}, \mathbf{y} \rangle - g^*(\mathbf{y})$$

**Examples:**  $g(\mathbf{z}) = \|\mathbf{z} - \mathbf{b}\|_1$ ,  $g(\mathbf{z}) = \|\mathbf{z} - \mathbf{b}\|_2^2$  or  $g(\mathbf{z}) = \iota_{\{\mathbf{b}\}}(\mathbf{z})$  (=0 if  $\mathbf{z} = \mathbf{b}$ ,  $+\infty$  otherwise) for which the Fenchel conjugate can be explicitly computed.

**Saddle Points** 

Consider the min-max problem:

 $(\mathbf{x}^*, \mathbf{y}^*)$  is a saddle point if  $\phi(\mathbf{x}^*, \mathbf{y}) \leq \phi(\mathbf{x}^*, \mathbf{y}^*) \leq$  $\phi(\mathbf{x}, \mathbf{y}^*)$  for any  $\mathbf{x} \in \mathcal{X}, \mathbf{y} \in \mathcal{Y}$ • Game interpretation: Nash equilibrium

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

• No player has the incentive to make unilateral change at NE. Simultaneous game **Global Minimax Points** 

• Game interpretation: Stackelberg equilibrium

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

 $\geq \max_{\mathbf{v} \in \mathcal{V}} \phi(\mathbf{x}^*, \mathbf{y}) \geq \min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \phi(\mathbf{x}, \mathbf{y})$ 

 $\max_{\mathbf{y} \in \mathcal{Y}} \min_{\mathbf{x} \in \mathcal{X}} \phi\left(\mathbf{x}, \mathbf{y}\right) \ge \min_{\mathbf{x} \in \mathcal{X}} \phi\left(\mathbf{x}, \mathbf{y}^*\right) \ge \phi\left(\mathbf{x}^*, \mathbf{y}^*\right)$ 

•  $\phi(\mathbf{x}, \mathbf{y})$  is concave in  $\mathbf{y} \in \mathcal{Y}$  for every fixed  $\mathbf{x} \in \mathcal{X}$ .

•  $\phi(\mathbf{x}, \mathbf{y})$  is  $\mu_1$ -strongly convex in  $\mathbf{x} \in \mathcal{X}$  for every

**Strongly-convex-strongly-concave function** 

**Convex-concave function** 

such that

 $(\mathbf{x}^*, \mathbf{y}^*)$  is a global minimax point if  $\phi(\mathbf{x}^*, \mathbf{y}) \leq$  $\phi(\mathbf{x}^*, \mathbf{y}^*) \le \max_{\mathbf{y}' \in \mathcal{Y}} \phi(\mathbf{x}, \mathbf{y}') \text{ for any } \mathbf{x} \in \mathcal{X}, \mathbf{y} \in \mathcal{Y}$ 

 Best response to the best response. • Sequential game **Primal and Dual Problems** 

(P):  $\min \max \phi(\mathbf{x}, \mathbf{y}) := \min \phi(\mathbf{x})$  $\mathbf{x} \in \mathcal{X} \ \mathbf{y} \in \mathcal{Y}$ 

(D):  $\max_{\mathbf{y} \in \mathcal{Y}} \min_{\mathbf{x} \in \mathcal{X}} \phi(\mathbf{x}, \mathbf{y}) := \max_{\mathbf{y} \in \mathcal{Y}} \underline{\phi}(\mathbf{y})$ 

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

**Lemma 12.1 Characterization of Saddle Points**  $(\mathbf{x}^*, \mathbf{y}^*)$  is a saddle point iff

 $\Delta(I) =$ 

and  $\mathbf{x}^* \in \operatorname{argmin}_{\mathbf{x} \in \mathcal{X}} \overline{\phi}(\mathbf{x}), \ \mathbf{y}^* \in \operatorname{argmax}_{\mathbf{y} \in \mathcal{Y}} \phi(\mathbf{y})$ Invoking the definition of saddle point, we have

Let f, g be convex nonsmooth functions,  $\mathbf{A} \in \mathbb{R}^{p \times d}$  a

$$\min_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}) + g(\mathbf{A}\mathbf{x})$$

$$|\mathbf{z} - \mathbf{b}||_1, g(\mathbf{z}) = ||\mathbf{z} - \mathbf{b}||_2^2 \text{ or}$$

If  $\mathcal{X}$  and  $\mathcal{Y}$  are closed convex sets and one of them is bounded, and  $\phi(\mathbf{x}, \mathbf{y})$  is a continuous convex-concave function, then there exists a saddle point on  $\mathcal{X} \times \mathcal{Y}$ 

**Thm 12.4 Minimax Theorem** 

13.4 First-order Methods

 $\max_{\mathbf{y} \in \mathcal{Y}} \min_{\mathbf{x} \in \mathcal{X}} \phi(\mathbf{x}, \mathbf{y}) = \min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \phi(\mathbf{x}, \mathbf{y})$ Here **x**, **y** are arbitrary values, not necessarily a sadd-

**Duality Gap: Accuracy Measure of Minimax Optimi-**

For convex-concave minimax optimization, saddle points exist. We measure the optimality via the duality gap.

duality gap :=  $\max_{\mathbf{y} \in \mathcal{V}} \phi(\hat{\mathbf{x}}, \mathbf{y}) - \min_{\mathbf{x} \in \mathcal{X}} \phi(\mathbf{x}, \hat{\mathbf{y}}) \ge 0$ .

le point.

• When duality gap = 0,  $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$  is a saddle point. • When duality gap  $\leq \epsilon$ ,  $(\hat{\mathbf{x}}, \hat{\mathbf{y}})$  is an  $\epsilon$ -saddle point.

**Gradient Descent Ascent (GDA)** 

 $\mathbf{x}_{t+1} = \prod_{\mathcal{X}} (\mathbf{x}_t - \gamma \nabla_{\mathbf{x}} \phi (\mathbf{x}_t, \mathbf{y}_t))$  $\mathbf{y}_{t+1} = \Pi_{\mathcal{V}} \left( \mathbf{y}_t + \gamma \nabla_{\mathbf{v}} \phi \left( \mathbf{x}_t, \mathbf{y}_t \right) \right)$ 

Strongly-Convex-Strongly-Concave (SC-SC) Setting • μ-strongly convex about **x** and strongly concave

 $\phi(\mathbf{x}_1,\mathbf{y}) \geq \phi(\mathbf{x}_2,\mathbf{y}) + \nabla_{\mathbf{x}}\phi(\mathbf{x}_2,\mathbf{y})^{\top}(\mathbf{x}_1 - \mathbf{x}_2)$ 

 $\|\nabla_{\mathbf{x}}\phi(\mathbf{x}_1,\mathbf{y}_1) - \nabla_{\mathbf{x}}\phi(\mathbf{x}_2,\mathbf{y}_2)\|$ 

 $\|\nabla_{\mathbf{v}}\phi(\mathbf{x}_1,\mathbf{y}_1) - \nabla_{\mathbf{v}}\phi(\mathbf{x}_2,\mathbf{y}_2)\|$ 

 $\leq L(||\mathbf{x}_1 - \mathbf{x}_2|| + ||\mathbf{y}_1 - \mathbf{y}_2||)$ 

 $\leq L(||\mathbf{x}_1 - \mathbf{x}_2|| + ||\mathbf{y}_1 - \mathbf{y}_2||)$ 

 $+\frac{\mu}{2}||\mathbf{x}_1-\mathbf{x}_2||^2$  $-\phi\left(\mathbf{x}_{1},\mathbf{y}_{1}\right) \geq -\phi\left(\mathbf{x},\mathbf{y}_{2}\right) - \nabla_{\mathbf{v}}\phi\left(\mathbf{x},\mathbf{y}_{2}\right)^{\top}\left(\mathbf{y}_{1}-\mathbf{y}_{2}\right)$  $+\frac{\mu}{2}||\mathbf{y}_1-\mathbf{y}_2||^2$ 

• *l*-Lipschitz smooth jointly in **x** and **y**:

13.3 Convex-Concave Min-Max Optimization

A function  $\phi(\mathbf{x}, \mathbf{y}) : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$  is convex-concave if •  $\phi(\mathbf{x}, \mathbf{y})$  is convex in  $\mathbf{x} \in \mathcal{X}$  for every fixed  $\mathbf{y} \in \mathcal{Y}$ ;

A function  $\phi(\mathbf{x}, \mathbf{y}) : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$  is strongly-convexstrongly-concave if there exist constants  $\mu_1, \mu_2 > 0$ 

 There exists a unique saddle point (x\*, y\*) Thm 12.5 Convergence of GDA for SC-SC Setting

In SC-SC setting, GDA with stepsize  $\eta < \frac{\mu}{2L^2}$  converges linearly:

 $\|\mathbf{x}_{t+1} - \mathbf{x}^*\|^2 + \|\mathbf{y}_{t+1} - \mathbf{y}^*\|^2$ 

•  $\phi(\mathbf{x}, \mathbf{y})$  is  $\mu_2$ -strongly concave in  $\mathbf{y} \in \mathcal{Y}$  for every fixed  $\mathbf{x} \in \mathcal{X}$ .

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When 
$$\eta = \frac{\mu}{4L^2}$$
,  
 $\|\mathbf{x}_T - \mathbf{x}^*\|^2 + \|\mathbf{y}_T - \mathbf{y}^*\|^2$   
 $\leq (1 - 4\mu^2/L^2)^{\top} (\|\mathbf{x}_0 - \mathbf{x}^*\|^2 + \|\mathbf{y}_0 - \mathbf{y}^*\|^2)$ 

It implies a complexity of  $\mathcal{O}(\kappa^2 \log \frac{1}{\epsilon})$  with  $\kappa = L/\mu$ being condition number.

#### Extragradient (EG)

$$\begin{split} &\mathbf{x}_{t+\frac{1}{2}} = \Pi_{\mathcal{X}}\left(\mathbf{x}_{t} - \eta \nabla_{\mathbf{x}}\phi\left(\mathbf{x}_{t}, \mathbf{y}_{t}\right)\right) \\ &\mathbf{y}_{t+\frac{1}{2}} = \Pi_{\mathcal{Y}}\left(\mathbf{y}_{t} + \eta \nabla_{\mathbf{y}}\phi\left(\mathbf{x}_{t}, \mathbf{y}_{t}\right)\right) \\ &\mathbf{x}_{t+1} = \Pi_{\mathcal{X}}\left(\mathbf{x}_{t} - \eta \nabla_{\mathbf{x}}\phi\left(\mathbf{x}_{t+\frac{1}{2}}, \mathbf{y}_{t+\frac{1}{2}}\right)\right) \\ &\mathbf{y}_{t+1} = \Pi_{\mathcal{Y}}\left(\mathbf{y}_{t} + \eta \nabla_{\mathbf{y}}\phi\left(\mathbf{x}_{t+\frac{1}{2}}, \mathbf{y}_{t+\frac{1}{2}}\right)\right) \end{split}$$

#### Thm 12.6 EG for C-C Setting

Assume  $\phi$  is convex-concave, L-Lipschitz smooth,  $\mathcal{X}$ has diameter  $D_{\mathcal{X}}$ , and  $\mathcal{Y}$  has diameter  $D_{\mathcal{V}}$ , then EGwith stepsize  $\eta \leq \frac{1}{2T}$  satisfies

 $\mathcal{O}(1/T)$  convergence rate for averaged iterates at "mid-point".

 $\mathcal{O}(1/T)$  rate is optimal.

In SC-SC setting, EG with stepsize  $\eta = \frac{1}{8L}$  converges linearly:

$$\|\mathbf{x}_{t+1} - \mathbf{x}^*\|^2 + \|\mathbf{y}_{t+1} - \mathbf{y}^*\|^2 \le \left(1 - \frac{\mu}{4L}\right) \left\{ \|\mathbf{x}_t - \mathbf{x}^*\|^2 + \|\mathbf{y}_t - \mathbf{y}^*\|^2 \right\}$$

This  $\mathcal{O}(\kappa \log \frac{1}{\epsilon})$  complexity is optimal for SC-SC set- • (Strong) solution (of Stampacchia VI): find  $\mathbf{z}^* \in$ 

#### **Optimistic GDA**

$$\mathbf{x}_{t+\frac{1}{2}} = \Pi_{\mathcal{X}} \left( \mathbf{x}_{t} - \eta \nabla_{\mathbf{x}} \phi \left( \mathbf{x}_{t-\frac{1}{2}}, \mathbf{y}_{t-\frac{1}{2}} \right) \right)$$

$$\mathbf{y}_{t+\frac{1}{2}} = \Pi_{\mathcal{Y}} \left( \mathbf{y}_{t} + \eta \nabla_{\mathbf{y}} \phi \left( \mathbf{x}_{t-\frac{1}{2}}, \mathbf{y}_{t-\frac{1}{2}} \right) \right)$$

$$\mathbf{x}_{t+1} = \Pi_{\mathcal{X}} \left( \mathbf{x}_{t} - \eta \nabla_{\mathbf{x}} \phi \left( \mathbf{x}_{t+\frac{1}{2}}, \mathbf{y}_{t+\frac{1}{2}} \right) \right)$$

$$\mathbf{y}_{t+1} = \Pi_{\mathcal{Y}} \left( \mathbf{y}_{t} + \eta \nabla_{\mathbf{y}} \phi \left( \mathbf{x}_{t+\frac{1}{2}}, \mathbf{y}_{t+\frac{1}{2}} \right) \right)$$

Equivalent formulation:

$$\begin{cases} \mathbf{x}_{t+1} = \mathbf{x}_t - 2\eta \nabla_{\mathbf{x}} \phi\left(\mathbf{x}_t, \mathbf{y}_t\right) + \eta \nabla_{\mathbf{x}} \phi\left(\mathbf{x}_{t-1}, \mathbf{y}_{t-1}\right) \\ \mathbf{y}_{t+1} = \mathbf{y}_t - 2\eta \nabla_{\mathbf{y}} \phi\left(\mathbf{x}_t, \mathbf{y}_t\right) + \eta \nabla_{\mathbf{y}} \phi\left(\mathbf{x}_{t-1}, \mathbf{y}_{t-1}\right) \end{cases}$$

**Proximal Point Algorithm (PPA)** 

$$(\mathbf{x}_{t+1}, \mathbf{y}_{t+1}) \leftarrow \underset{\mathbf{x} \in \mathcal{X}}{\operatorname{argmax}} \left\{ \phi(\mathbf{x}, \mathbf{y}) + \frac{1}{2\eta} \|\mathbf{x} - \mathbf{x}_t\|^2 - \frac{1}{2\eta} \|\mathbf{y} - \mathbf{y}_t\|^2 \right\}$$

PPA has been shown to converge with  $\mathcal{O}(1/T)$  rate in convex-concave case. **Implicit Update of PPA** 

$$\mathbf{x}_{t+1} = \Pi_{\mathcal{X}} \left( \mathbf{x}_{t} - \eta \nabla_{\mathbf{x}} \phi \left( \mathbf{x}_{t+1}, \mathbf{y}_{t+1} \right) \right)$$
  
$$\mathbf{y}_{t+1} = \Pi_{\mathcal{Y}} \left( \mathbf{y}_{t} + \eta \nabla_{\mathbf{y}} \phi \left( \mathbf{x}_{t+1}, \mathbf{y}_{t+1} \right) \right)$$

#### **Connections between PPA, EG and OGDA** Handout13 Page 33

13.5 Concave Games, Variational Inequalities

#### Variational Inequality Problem (VI)

Let  $\mathcal{Z} \subset \mathbb{R}^d$  be a nonempty subset and consider a mapping  $F: \mathcal{Z} \to \mathbb{R}^d$ .

**VI Problem:** Find  $\mathbf{z}^* \in \mathcal{Z}$  such that  $\langle F(\mathbf{z}^*), \mathbf{z} - \mathbf{z}^* \rangle \geq 0$ 

**Existence:** If  $\mathcal{Z}$  is a nonempty convex compact subset of  $\mathbb{R}^d$  and  $F: \mathbb{Z} \to \mathbb{R}^d$  is continuous, then there

monotone if

$$\langle F(\mathbf{u}) - F(\mathbf{v}), \mathbf{u} - \mathbf{v} \rangle \ge 0 \quad \forall \mathbf{u}, \mathbf{v} \in \mathcal{Z}$$

• u-strongly-monotone (u > 0) if

$$\langle F(\mathbf{u}) - F(\mathbf{v}), \mathbf{u} - \mathbf{v} \rangle \ge \mu ||\mathbf{u} - \mathbf{v}||^2 \quad \forall \mathbf{u}, \mathbf{v} \in \mathcal{Z}$$

#### **Weak Solution of VI**

 $\mathcal{Z}$  such that:

$$\langle F(\mathbf{z}^*), \mathbf{z} - \mathbf{z}^* \rangle \ge 0 \,\forall \mathbf{z} \in \mathcal{Z}.$$

• Weak solution (of Minty VI): find  $z^* \in \mathcal{Z}$  such

$$\langle F(\mathbf{z}), \mathbf{z} - \mathbf{z}^* \rangle \ge 0 \,\forall \mathbf{z} \in \mathcal{Z}.$$

- If F is monotone, then a strong solution is also a weak solution.
- If F is continuous, then a weak solution is also a strong solution.
- We use  $\epsilon_{VI}(\hat{\mathbf{z}}) := \max_{\mathbf{u} \in \mathcal{Z}} \langle F(\mathbf{u}), \mathbf{u} \hat{\mathbf{z}} \rangle$  to measure the inaccuracy of a solution  $\hat{\mathbf{z}}$ .