# First order methods

FOR CONVEX OPTIMIZATION

Saketh (IIT Bombay)

### **Topics**

- Part I
  - Optimal methods for unconstrained convex programs
    - Smooth objective
    - Non-smooth objective
- Part II
  - Optimal methods for constrained convex programs
    - Projection based
    - Frank-Wolfe based
    - Functional constraint based
  - Prox-based methods for structured non-smooth programs

# Non-Topics

- Step-size schemes
- Bundle methods
- Stochastic methods
- Inexact oracles
- Non-Euclidean extensions (Mirror-friends)

# Motivation

& EXAMPLE APPLICATIONS

• **Goal:** Construct  $f: X \to Y$ 

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- Model:  $f(x) = w^T \phi(x)$
- Algorithm: Find simple functions that explain data

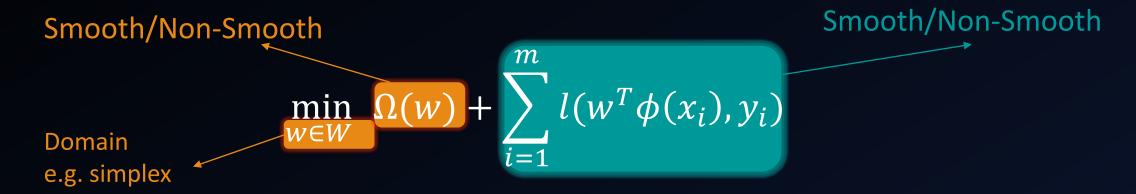
$$\min_{w \in R^n} \Omega(w) + \sum_{i=1}^m l(w^T \phi(x_i), y_i)$$

# Typical Program – Machine Learning

Smooth/Non-Smooth  $\min_{w \in R^n} \Omega(w) + \sum_{i=1}^m l(w^T \phi(x_i), y_i)$ 

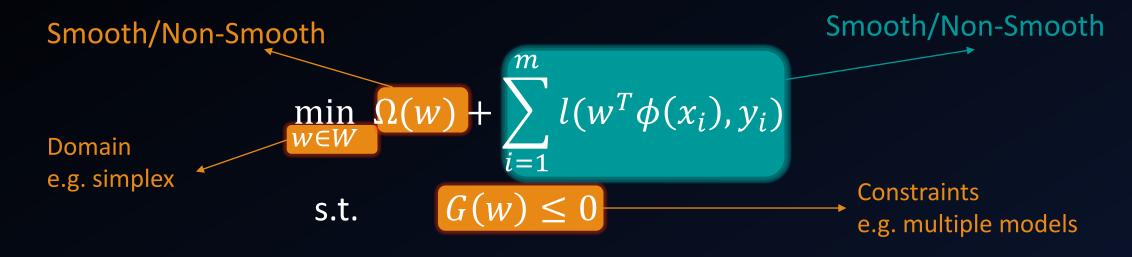
- Unconstrained
  - , smooth functional constraints
- Smooth/Non-smooth/Composite Objectives

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#### Scale is the issue!

- m, n as well as no. models may run into millions!
- Even a single iteration of IPM/Newton-variants is in-feasible.
- "Slower" but "cheaper" methods are the alternative
  - Decomposition based
  - First order methods

#### First Order Methods - Overview

- Iterative, gradient-like information, O(n) per iteration
- E.g. Gradient method, Cutting planes, Conjugate gradient
- Very old methods (1950s)
- Far slower than IPM
  - Sub-linear rate ® . (Not crucial for ML)
  - But (nearly) n-independent ©
- Widely employed in state-of-the-art ML systems
- Choice of variant depends on problem structure

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# Smooth un-constrained

$$\underset{w \in \mathbb{R}^n}{\text{MIN}} \sum_{i=1}^m (w^T \phi(x_i) - y_i)^2$$

- Continuously differentiable
- Gradient is Lipschitz continuous

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  - $\|\nabla f(x) \nabla f(y)\| \le L\|x y\|$
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  - E.g.  $g(x) \equiv |x|$  is L-conts. with L=1

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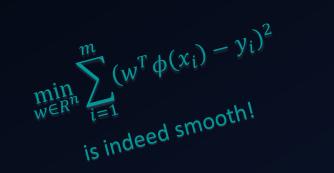
**Theorem:** Let f be convex twice differentiable. Then

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# Gradient Method [Cauchy1847]

- Move iterate in direction of instantaneous decrease
  - $x_{k+1} = x_k s_k \nabla f(x_k)$ ,  $s_k > 0$



#### **Gradient Method**

Move iterate in direction of instantaneous decrease

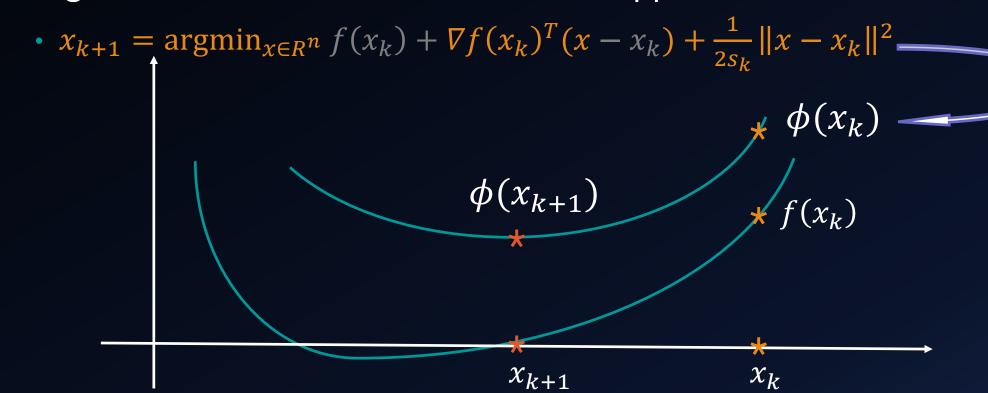
• 
$$x_{k+1} = x_k - s_k \nabla f(x_k)$$
,  $s_k > 0$ 

Regularized minimization of first order approx.

• 
$$x_{k+1} = \operatorname{argmin}_{x \in \mathbb{R}^n} f(x_k) + \nabla f(x_k)^T (x - x_k) + \frac{1}{2s_k} ||x - x_k||^2$$

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- Various step-size schemes
  - Constant (1/L)
  - Diminishing  $(s_k \downarrow 0, \sum s_k = \infty)$
  - Exact or back-tracking line search

# Convergence rate – Gradient method

**Theorem[NeO4]:** If f is smooth with const. L and  $s_k = \frac{1}{L}$ , then gradient method generates  $x_k$  such that:

$$f(x_k) - f(x^*) \le \frac{2L||x_0 - x^*||^2}{k+4}.$$

Proof Sketch.

- $f(x_{k+1}) \le f(x_k) + \nabla f(x_k)^T (x_{k+1} x_k) + \frac{L}{2} ||x_{k+1} x_k||^2$
- $f(x_{k+1}) \ge f(x_k) + \nabla f(x_k)^T (x_{k+1} x_k) + \frac{1}{2L} \|\nabla f(x_{k+1}) \nabla f(x_k)\|^2$
- $||x_{k+1} x^*||^2 \le ||x_k x^*||^2 \frac{1}{12} ||\nabla f(x_k)||^2$
- $\Delta_{k+1} \leq \Delta_k \Delta^2/_{2}$  (Solve recursion)

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Majorization minimization

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• 
$$||x_{k+1} - x^*||^2 \le ||x_k - x^*||^2 - \frac{1}{L^2} ||\nabla f(x_k)||^2$$

•  $\Delta_{k+1} \leq \Delta_k - \Delta^2/r_0^2$  (Solve recursion)

- Sub-linear, very slow compared to IPM
- Applies to conjugate gradient and other traditional variants
- Sub-optimal (may be?):

**Theorem[Ne04]:** For any  $k \leq \frac{n-1}{2}$ , and any  $x_0$ , there exists a smooth function f, with const. L, such that with any first order method, we have  $f(x_k) - f(x^*) \geq \frac{3L||x_0 - x^*||^2}{32(k+1)^2}.$ 

*Proof Sketch:* Choose function such that  $x_k \in lin(\nabla f(x_0), ..., \nabla f(x_{k-1})) \subset R^{k,r}$ 

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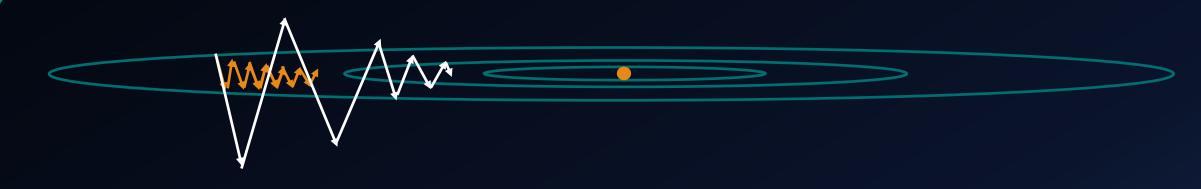
# Intuition for non-optimality

- All variants are descent methods
- Descent essential for proof
- Overkill leading to restrictive movements
- Try non-descent alternatives!



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# Towards optimality [Moritz Hardt]

Sub-optimal:  $O\left(\left(1-\frac{1}{Q}\right)^k\right)$ 

• 
$$f(x) = \frac{1}{2}x^{T}Ax - bx$$
;  $x_0 = b$ 

• 
$$x_k = x_{k-1} - \frac{1}{L}(Ax_{k-1} - b) = \sum_{i=0}^k \left(I - \frac{A}{L}\right)^i \frac{b}{L}$$

Chebyshev poly, have two term recursive formula, hence we expect:

•  $x_k = x_{k-1} - s_{k-1} \nabla f(x_{k-1}) + \lambda_{k-1} \nabla f(x_{k-2})$ , to be optimal (acceleration

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**Lemma[Mo12]:** There is a (Chebyshev) poly. of degree  $O(\sqrt{Q} \log^{1}/\epsilon)$  such that p(0) = 1 and  $p(x) \le \epsilon \ \forall \ x \in [\mu, L]$ .

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#### Accelerated Gradient Method [Ne83,88,Be09]

• 
$$y_k = x_{k-1} + \frac{k-2}{k+1}(x_{k-1} - x_{k-2})$$
 Two step history

• 
$$x_k = y_k - s_k \nabla f(y_k)$$

(Usual gradient step)

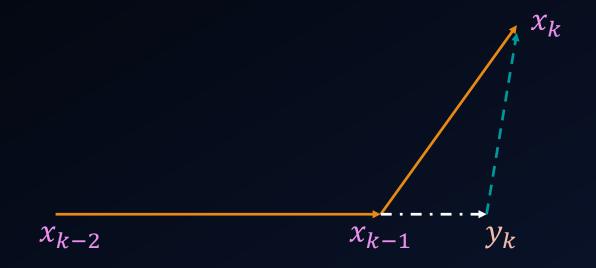
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(Extrapolation or momentum)

(Usual gradient step)



### Rate of Convergence – Accelerated gradient

**Theorem [Be09]:** If f is smooth with const. L and  $s_k = \frac{1}{L}$ , then accelerated gradient method generates  $x_k$  such that:

$$f(x_k) - f(x^*) \le \frac{2L||x_0 - x^*||^2}{(k+1)^2}.$$

Indeed optimal!

Proof Sketch.

- $f(x_k) \le f(z) + L(x_k y)^T (z x_k) + \frac{L}{2} ||x_k y||^2 \ \forall \ z \in \mathbb{R}^n$
- Convex combination at  $z=x_k, z=x^*$  leads to:

$$\frac{(k+1)^{2}}{2L}(f(x_{k}) - f^{*}) + \|\overline{y}_{k} - x^{*}\|^{2} \le \frac{(k)^{2}}{2L}(f(x_{k-1}) - f^{*}) + \|\overline{y}_{k-1} - x^{*}\|^{2}$$

$$\le \|x_{0} - x^{*}\|^{2}$$

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• Convex combination at  $z = x_k$ ,  $z = x^*$  leads to:

$$\frac{(k+1)^{2}}{2L}(f(x_{k})-f^{*})+\|\overline{y}_{k}-x^{*}\|^{2} \leq \frac{(k)^{2}}{2L}(f(x_{k-1})-f^{*})+\|\overline{y}_{k-1}-x^{*}\|^{2}$$

$$\leq \|x_{0}-x^{*}\|^{2}$$

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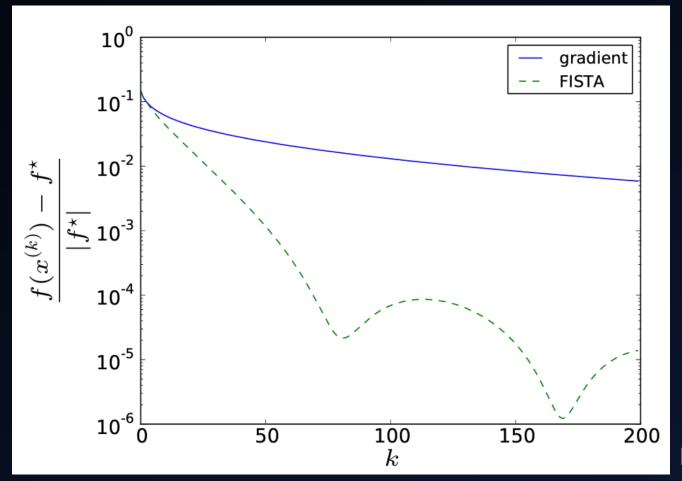
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$$\le \|x_{0} - x^{*}\|^{2}$$

### A Comparison of the two gradient methods

$$\min_{x \in R^{1000}} \log \left( \sum_{i=1}^{2000} e^{(a_i^T x + b_i)} \right)$$



### Junk variants other than Accelerated gradient?

- Accelerated gradient is
  - Less robust than gradient method [Moritz Hardt]
  - Accumulates error with inexact oracles [De13]
- Who knows what will happen in your application?

## Summary of un-constrained smooth convex programs

- Gradient method and friends:  $\epsilon \approx O(1/k)$ 
  - Sub-linear and sub-optimal rate.
  - Additionally, strong convexity gives:  $\epsilon \approx O\left(\left(\frac{Q-1}{Q+1}\right)^{2k}\right)$ . Sub-optimal but linear rate.
- Accelerated gradient methods:  $\epsilon \approx O(1/k^2)$ 
  - Sub-linear but optimal
  - O(n) computation per iteration
  - Additionally, strong convexity gives:  $\epsilon \approx O\left(\left(\frac{\sqrt{Q}-1}{\sqrt{Q}+1}\right)^{2R}\right)$ . Optimal but still linear rate.

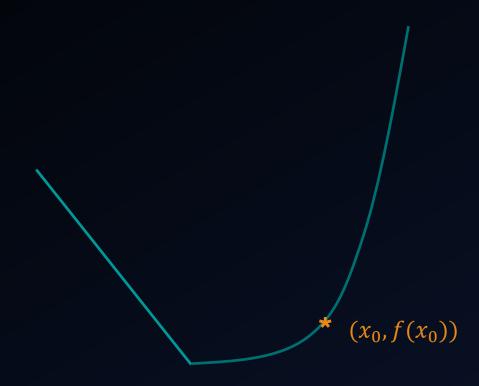
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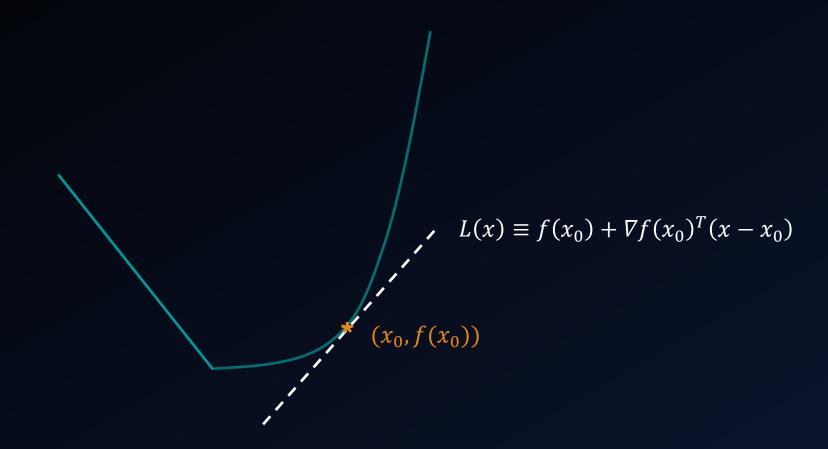
# Non-smooth unconstrained

$$\underset{w \in \mathbb{R}^n}{\text{MIN}} \sum_{i=1}^m |w'\phi(x_i) - y_i|$$

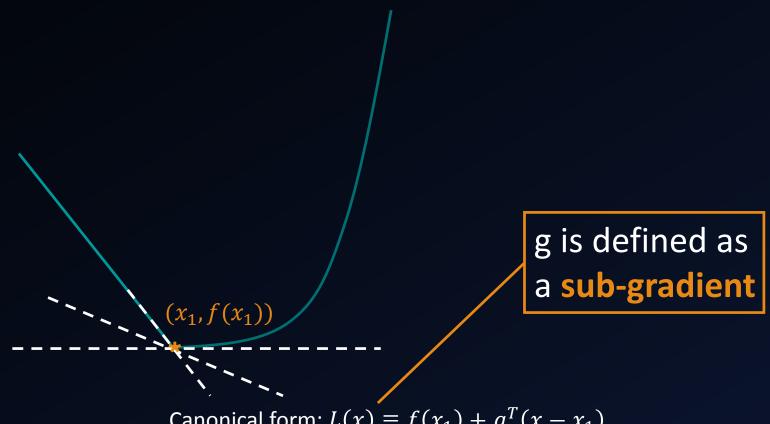
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Canonical form:  $L(x) \equiv f(x_1) + g^T(x - x_1)$ . Multiple g exist such that  $L(x) \leq f(x) \ \forall x$ 

### First Order Methods (Non-smooth)

**Theorem:** Let f be a closed convex function. Then

- At any  $x \in ri(dom f)$ , sub-gradient exists and set of all sub-gradients (denoted by  $\partial f(x)$ ; sub-differential set) is closed convex.
- If f is differentiable at  $x \in int(dom f)$ , then gradient is the only subgradient.

**Theorem:**  $x \in \mathbb{R}^n$  minimizes f if and only if  $0 \in \partial f(x)$ .

### Sub-gradient Method

- Assume oracle that throws a sub-gradient.
- Sub-gradient method:

• 
$$x_{k+1} = \operatorname{argmin}_{x \in \mathbb{R}^n} f(x_k) + g_f(x_k)^T (x - x_k) + \frac{1}{2s_k} ||x - x_k||^2$$

$$\bullet \ x_{k+1} = x_k - s_k g_f(x_k)$$

## Can sub-gradient replace gradient?

- No majorization minimization
- $-g_f(x)$  not even descent direction

• E.g. 
$$f(x_1, x_2) \equiv |x_1| + 2|x_2|$$



(1,0)

Expect slower than O(1/k)

How far can sub-gradient take?

### How far can sub-gradient take?

Always exists!

**Theorem[Ne04]:** Let  $||x_0 - x^*|| \le R$  and L the Lip. const. of f over this ball. Then sequence generated by sub-gradient descent satisfies:

$$\min_{i \in \{1,...,k\}} f(x_i) - f(x^*) \le \frac{LR}{\sqrt{k+1}}.$$

Proof Sketch:

- $2s_k \Delta_k \le r_k^2 r_{k+1}^2 + s_k^2 |g_f(x_k)|$
- LHS  $\leq \frac{r_0 + 2i = 0}{2} \frac{s_i ||g_f(x_k)||}{2 \sum_{i=0}^k s_i} \leq \frac{R^2 + \sum_{i=0}^n s_i^{-L}}{2 \sum_{i=0}^k s_i}$ ; Choose  $s_k = \frac{R}{\sqrt{k+1}}$

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#### Proof Sketch:

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$$2s_k \Delta_k \le r_k^2 - r_{k+1}^2 + s_k^2 \|g_f(x_k)\|^2$$

• LHS 
$$\leq \frac{r_0^2 + \sum_{i=0}^k s_i^2 \|g_f(x_k)\|^2}{2\sum_{i=0}^k s_i} \leq \frac{R^2 + \sum_{i=0}^k s_i^2 L^2}{2\sum_{i=0}^k s_i}$$
; Choose  $s_k = R/\sqrt{k+1}$ 

### Is this optimal?

**Theorem[Ne04]:** For any  $k \le n - 1$ , and any  $x_0$  such that

 $||x_0 - x^*|| \le R$ , there exists a convex f, with const. L over the ball, such that with any first order method, we have:

$$f(x_k) - f(x^*) \ge \frac{LR}{2(1 + \sqrt{k+1})}.$$

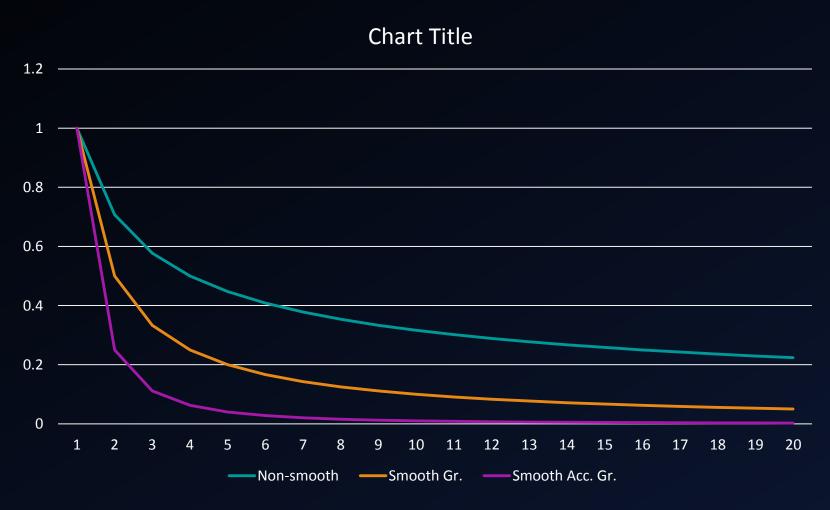
**Proof Sketch:** Choose function such that

$$x_k \in lin\left(g_f(x_0), \dots, g_f(x_{k-1})\right) \subset R^{k,n}$$

### Summary of non-smooth unconstrained

- Sub-gradient descent method:  $\epsilon \approx O\left(\frac{1}{\sqrt{k}}\right)$ .
  - Sub-linear, slower than smooth case
  - But, optimal!
  - Can do better if additional structure (later)

### Summary of Unconstrained Case



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