Adaptive Optimization Methods for Machine Learning and Signal Processing

Volkan Cevher
volkan.cevher@epfl.ch

Ali Kavis
ali.kavis@epfl.ch

Kfir Y. Levy
kfirylevy@technion.ac.il

Ahmet Alacaoglu
ahmet.alacaoglu@epfl.ch

Part I/IV: An introduction

Laboratory for Information and Inference Systems (LIONS)
École Polytechnique Fédérale de Lausanne (EPFL)

Further acknowledgements

- LIONS group members (current & alumni): https://lions.epfl.ch
  - EE-556 (Mathematics of Data): Course material
- Optimization for Machine Learning (OPT-ML) 2020 Workshop at NeurIPS: https://opt-ml.org/

One formula to rule all ML & SP problems

$$f^\star = \min_{x : x \in \mathcal{X}} f(x) \quad (\text{argmin} \rightarrow x^\star)$$

◦ Growing interest in first-order gradient methods[1] due to their scalability and generalization performance

[1] Lan, Guanghui. First-order and Stochastic Optimization Methods for Machine Learning. Springer Nature, 2020.

One formula to rule ~~all~~ some ML & SP problems ...and one algorithm to solve them.

$$f^\star = \min_{x : x \in \mathcal{X}} f(x) \quad (\text{argmin} \to x^\star)$$

- Growing interest in first-order gradient methods[1] due to their scalability and generalization performance
- In the sequel, the set $\mathcal{X}$ is convex:
  - $\forall x, y \in \mathcal{X} \quad \forall \alpha \in [0,1], \quad \alpha x + (1-\alpha) y \in \mathcal{X}.$
- In the sequel, the function f may be convex:
  - $f(\alpha x + (1-\alpha) y) \leq \alpha f(x) + (1-\alpha) f(y), \qquad \forall x, y \in \mathcal{X}, \quad \forall \alpha \in [0,1].$

[1] Lan, Guanghui. First-order and Stochastic Optimization Methods for Machine Learning. Springer Nature, 2020.

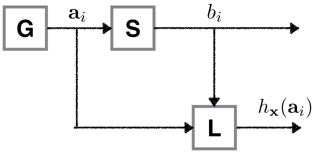
One formula to rule ~~all~~ some ML & SP problems ...and one algorithm to solve them.

$$f^\star = \min_{x:x\in\mathcal{X}} f(x) \quad (\text{argmin} \to x^\star)$$

- Growing interest in first-order gradient methods[1] due to their scalability and generalization performance
- In the sequel, the set $\mathcal{X}$ is convex:
  - $\forall x, y \in \mathcal{X} \quad \forall \alpha \in [0,1], \quad \alpha x + (1-\alpha) y \in \mathcal{X}.$
- In the sequel, the function f may not be convex:
  - $f(\alpha x + (1-\alpha) y) \not\leq \alpha f(x) + (1-\alpha) f(y), \qquad \forall x, y \in \mathcal{X}, \quad \forall \alpha \in [0,1].$

[1] Lan, Guanghui. First-order and Stochastic Optimization Methods for Machine Learning. Springer Nature, 2020.

Application: Deep learning via empirical risk minimization



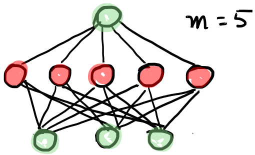
Definition (Optimization formulation)

The deep-learning training problem is given by

$$x^\star_{\mathsf{DL}} \in \arg\min_{x \in \mathcal{X}} \left\{ f(x) := \frac{1}{n} \sum_{i=1}^{n} L(h_x(\mathbf{a}_i), b_i) \right\},$$

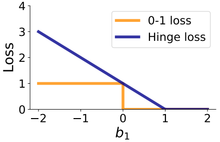
where $\mathcal{X}$ denotes the constraints on the parameters.

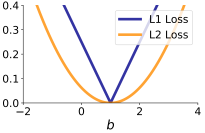
◦ A single hidden layer neural network with params $x := [\mathbf{X}_1, \mathbf{X}_2, \mu_1, \mu_2]$

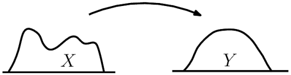


$$h_x(\mathbf{a}) := \Big[\ \mathbf{X}_2\ \Big]\ \underbrace{\overset{\text{activation}}{\sigma} \Big(\Big[\ \overset{\text{weight}}{\mathbf{X}_1}\ \Big] \Big[\overset{\text{input}}{\mathbf{a}}\Big] + \Big[\overset{\text{bias}}{\mu_1}\Big] \Big) + \Big[\overset{\text{bias}}{\mu_2}\Big]}_{\text{hidden layer = learned features}}$$

Loss function examples







Definition (Hinge loss)

For a binary classification problem, the hinge loss for a score value $b_1 \in \mathbb{R}$ and class label $b_2 \in \pm 1$ is given by $L(b_1, b_2) = \max(0, 1 - b_1 \times b_2)$.

Definition (ℓ_q-losses)

For all $b_1, b_2 \in \mathbb{R}^n \times \mathbb{R}^n$, we can use $L_q(b_1, b_2) = \|b_1 - b_2\|_q^q$, where

$$\ell_q\text{-norm:} \quad \|b\|_q^q := \sum_{i=1}^n |b_i|^q \quad \text{for } b \in \mathbb{R}^n \text{ and } q \in [1, \infty)$$

Definition (Wasserstein distance)

Let μ and ν be two probability measures on $\mathbb{R}^d$ an define their couplings as $\Gamma(\mu, \nu) := \{\pi \text{ probability measure on } \mathbb{R}^d \times \mathbb{R}^d \text{ with marginals } \mu, \nu\}$.

$$W(\mu, \nu) := \left(\inf_{\pi \in \Gamma(\mu,\nu)} \mathbb{E}_{(x,y)\sim\pi} \|x - y\|^2 \right)^{1/2}$$

A basic *iterative* strategy

$$f^\star = \min_{x : x \in \mathcal{X}} f(x) \quad (\text{argmin} \to x^\star)$$

General idea of an optimization algorithm

Guess a solution, and then *refine* it based on *oracle information*.

Repeat the procedure until the result is *good enough*.

Basic principles of descent methods

Template for iterative descent methods

1. Let $x_0 \in \mathcal{X}$ be a starting point.
2. Generate a sequence of vectors $x_1, x_2, \dots \in \mathcal{X}$ so that we have descent:

$$f(x_{t+1}) < f(x_t), \quad \text{for all } t = 0, 1, \dots$$

   until x_t satisfies $f(x_t) - f^\star \leq \epsilon$.

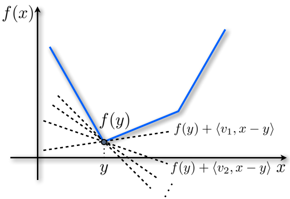
Such a sequence $\{x_t\}_{t \geq 0}$ can be generated as:

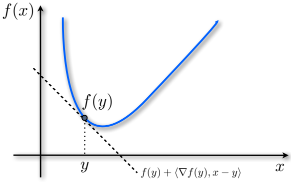
$$x_{t+1} = x_t + \alpha_t p_t$$

where p_t is a descent direction and $\alpha_t > 0$ a step-size.

Remarks:
- Iterative algorithms can use various **oracle** information in the optimization problem
- The type of oracle information used becomes a defining characteristic of the algorithm
- Example oracles: Objective value, gradient, and Hessian result in 0-th, 1-st, 2-nd order methods
- The oracle choices determine α_k and p_t as well as the overall convergence rate and complexity

First-order methods use subdifferentials & gradients





Definition (Subdifferential)

The subdifferential of f at x, denoted $\partial f(x)$, is the set of all vectors v satisfying

$$f(y) \geq f(x) + \langle v, y - x\rangle + o(\|y - x\|) \quad \text{as } y \to x.$$

If the function f is differentiable, then its subdifferential contains only the gradient.

Basic principles of descent methods ($\mathcal{X} = \mathbb{R}^p$)

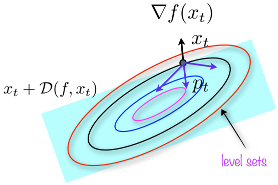


Figure: Descent directions in 2D should be an element of the cone of descent directions $\mathcal{D}(f, \cdot)$.

- Recall the representation of the algorithmic iterates:

$$x_{t+1} = x_t + \alpha_t p_t.$$

- For a differentiable f, apply Taylor's theorem with $\alpha_t = o(1)$

$$f(x_{t+1}) = f(x_t) + \alpha_t \langle \nabla f(x_t),\ p_t \rangle + \mathcal{O}(\alpha_t^2 \, \|p_t\|_2^2).$$

- To obtain $f(x_{t+1}) < f(x_t)$, we need $\langle \nabla f(x_t),\ p_t \rangle < 0$!

Observations:

- The local *steepest descent* direction is the negative gradient $p_t := -\nabla f(x_t)$
  - $\langle \nabla f(x_t),\ p_t \rangle = \|\nabla f(x_t)\| \|p_t\| \cos \theta$
  - θ is the angle between $\nabla f(x_t)$ and p_t
- We can use a subgradient $p_t \in -\partial f(x_t)$ as a descent direction

Brief detour: Gradients of vector valued functions

Jacobian

When $f : \mathbb{R}^n \rightrightarrows \mathbb{R}^d$ is a vector valued function, the following $d \times n$ matrix $\mathbf{J}$ of partial derivatives[1]

$$\left[\mathbf{J}_f(x)\right]_{i,j} := \frac{\partial f_i}{\partial x_j}(x)$$

is called the Jacobian of f at x.

Observations:

- The Jacobian is the transpose of the gradient, when f is real valued.
- Thinking in terms of Jacobians is really helpful when we need to use the chain rule.

Chain Rule via Jacobians

Let $\circ$ denote the functional composition: $g \circ f := g(f(x))$. If $g \circ f$ is differentiable at x, then the following holds

$$\mathbf{J}_{g\circ f}(x) = \mathbf{J}_g(f(x))\mathbf{J}_f(x).$$

Hence, the chain rule, which is helpful in differentiating function compositions, can be related to a simple product of Jacobian matrices.

[1] We overload the notation x_i to denote i^{th} coordinate when it is clear from the context. When we have x_t, we use $x_{t,i}$.

An example

Example

The gradient of $f : x \mapsto \boldsymbol{w}_2^\top \sigma(\mathbf{W}_1 x + \boldsymbol{\mu})$ is given by the following expression:

$$\nabla f(x) = \mathbf{J}_f(x)^\top = \mathbf{W}_1^\top (\sigma'(\mathbf{W}_1 x + \boldsymbol{\mu}) \odot \boldsymbol{w}_2),$$

where σ is a non-linear function that applies to each coordinate, and $\odot$ denotes the component wise product.

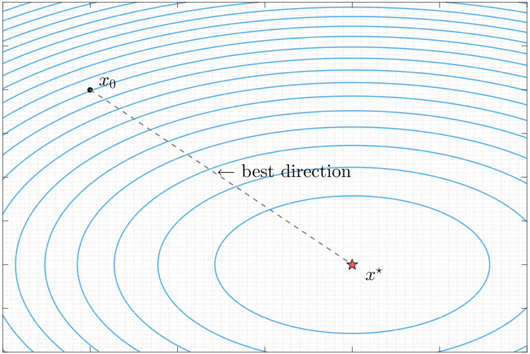
Proof: f is a composition of the functions $k \circ g \circ h$

- $h(x) = \mathbf{W}_1 x + \boldsymbol{\mu}$, whose Jacobian is $\mathbf{J}_h(x) = \mathbf{W}_1$.
- $g(x) = \begin{bmatrix} \sigma(x_1) \\ \vdots \\ \sigma(x_n) \end{bmatrix}$, whose Jacobian is $\mathbf{J}_g(x) = \text{diag}(\sigma'(x_1), \dots, \sigma'(x_n))$.
- $k(x) = \boldsymbol{w}_2^\top x$ whose Jacobian is $\mathbf{J}_k(x) = \boldsymbol{w}_2^\top$.
- By the chain rule, we have that

$$\begin{aligned} \mathbf{J}_f(x) &= \mathbf{J}_k(g(h(x))) \cdot \mathbf{J}_g(h(x)) \cdot \mathbf{J}_h(x) \\ &= \boldsymbol{w}_2^\top \cdot \text{diag}(\sigma'([\mathbf{W}_1 x + \boldsymbol{\mu}]_1), \dots, \sigma'([\mathbf{W}_1 x + \boldsymbol{\mu}]_n)) \cdot \mathbf{W}_1 \end{aligned}$$

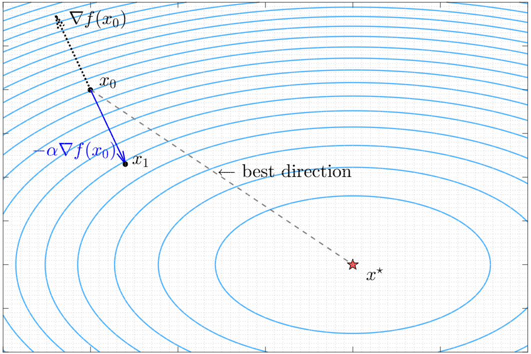
Simply transpose the Jacobian to get the gradient and use $\odot$ to replace the diagonal matrix.

A simple iterative algorithm: Gradient descent



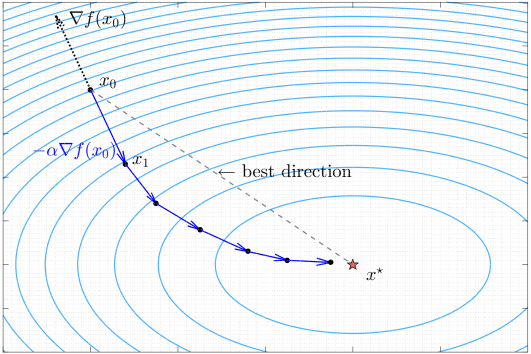
- Choose initial point: x_0.

A simple iterative algorithm: Gradient descent



- Choose initial point: x_0.
- Take a step in the negative gradient direction with a step size $\alpha > 0$: $x_{t+1} = x_t - \alpha\nabla f(x_t)$.

A simple iterative algorithm: Gradient descent



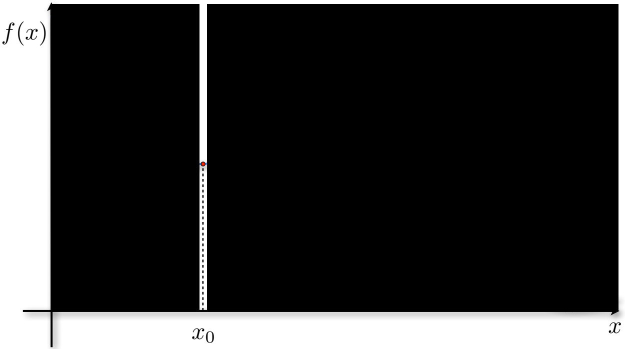
- Choose initial point: x_0.
- Take a step in the negative gradient direction with a step size $\alpha > 0$: $x_{t+1} = x_t - \alpha \nabla f(x_t)$.
- Repeat this procedure until x_t is accurate enough.

Challenges for an iterative optimization algorithm

Problem

Find the minimum $x^\star$ of $f(x)$, given starting point x_0 based on only local information.

- **Fog of war**

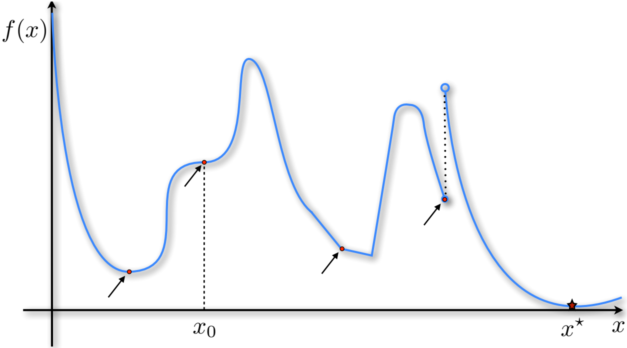


Challenges for an iterative optimization algorithm

Problem

Find the minimum $x^\star$ of $f(x)$, given starting point x_0 based on only local information.

- Fog of war, non-differentiability, discontinuities, local minima, stationary points...



A notion of convergence: Stationarity

- Let $f : \mathbb{R}^p \to \mathbb{R}$ be twice-differentiable and $x^\star = \min_{x \in \mathbb{R}^p} f(x)$

Gradient method

Choose a starting point x_0 and iterate

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

where $\alpha > 0$ is a step-size to be chosen so that x_t converges to $x^\star$.

Definition (First order stationary point (FOSP))

A point $\bar{x}$ is a first order stationary point of a twice differentiable function f if

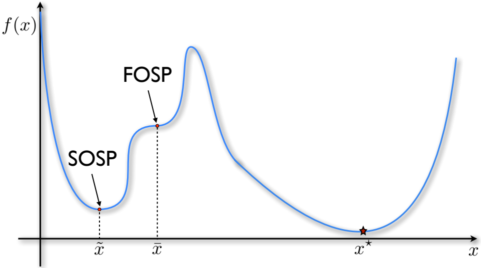
$$\nabla f(\bar{x}) = \mathbf{0}.$$

Fixed-point characterization

Multiply by -1 and add $\bar{x}$ to both sides to obtain the fixed point condition:

$$\bar{x} = \bar{x} - \alpha \nabla f(\bar{x}) \qquad \text{for all } \alpha \in \mathbb{R}.$$

Geometric interpretation of stationarity



Observation: ○ Neither $\bar{x}$, nor $\tilde{x}$ is **necessarily** equal to $x^\star$!!

Proposition (*Local minima, maxima, and saddle points)

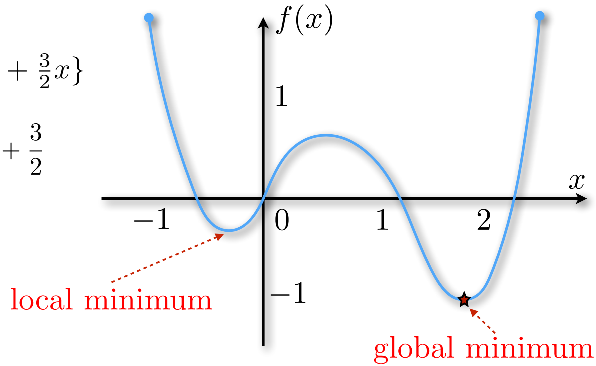
Let $\bar{x}$ be a stationary point of a twice differentiable function f.

- *If $\nabla^2 f(\bar{x}) \succ 0$, then the point $\bar{x}$ is called a local minimum or a second order stationary point (SOSP).*
- *If $\nabla^2 f(\bar{x}) \prec 0$, then the point $\bar{x}$ is called a local maximum.*
- *If $\nabla^2 f(\bar{x}) = 0$, then the point $\bar{x}$ can be a saddle point, a local minimum, or a local maximum.*

Local minima

$$\min_{x\in\mathbb{R}}\{x^4 - 3x^3 + x^2 + \tfrac{3}{2}x\}$$

$$\frac{df}{dx} = 4x^3 - 9x^2 + 2x + \frac{3}{2}$$



Choose $x_0 = 0$ and $\alpha = \frac{1}{6}$

$x_1 = x_0 - \alpha \frac{df}{dx}\big|_{x=x_0} = 0 - \frac{1}{6}\frac{3}{2} = -\frac{1}{4}$

$x_2 = -\frac{5}{16}$

...

x_t converges to a **local minimum**!

From local to global optimality

Definition (Local minimum)

Given $f : \mathbb{R}^p \to \mathbb{R} \cup \{+\infty\}$, a vector $x^\star \in \mathbb{R}^p$ is called a *local minimum* of f if there exists $\epsilon > 0$ s.t.

$$f(x^\star) \leq f(x) \quad \forall x \in \mathbb{R}^p \quad \text{with} \quad \|x - x^\star\| \leq \epsilon.$$

Theorem

If $\mathcal{Q} \subset \mathbb{R}^p$ is a convex set and $f : \mathbb{R}^p \to (-\infty, +\infty]$ is a proper convex function, then a local minimum of f over $\mathcal{Q}$ is also a global minimum of f over $\mathcal{Q}$.

Proof.

Suppose $x^\star$ is a local minimum but not global, i.e. there exist $x \in \mathbb{R}^p$ s.t. $f(x) < f(x^\star)$. By convexity,

$$f(\alpha x^\star + (1-\alpha)x) \leq \alpha f(x^\star) + (1-\alpha) f(x) < f(x^\star), \forall \alpha \in [0, 1]$$

which contradicts the local minimality of $x^\star$. □

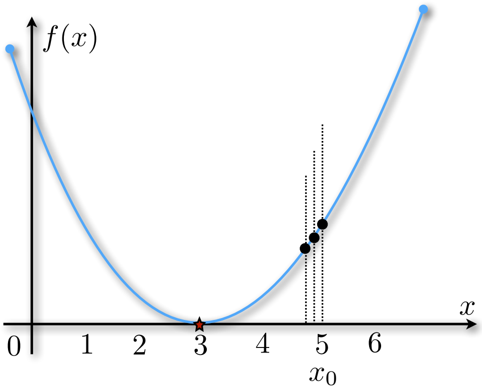
Theorem

Let $f : \mathbb{R}^p \to \mathbb{R}$ be a convex differentiable function. Then any stationary point of f is a global minimum.

Effect of very small step-size α...

$$\min_{x \in \mathbb{R}} \frac{1}{2}(x-3)^2$$

$$\frac{df}{dx} = x - 3$$



Choose $x_0 = 5$ and $\boldsymbol{\alpha = \frac{1}{10}}$

$x_1 = x_0 - \alpha \frac{df}{dx}\Big|_{x=x_0} = 5 - \frac{1}{10}2 = 4.8$

$x_2 = x_1 - \alpha \frac{df}{dx}\Big|_{x=x_1} = 4.8 - \frac{1}{10}1.8 = 4.62$

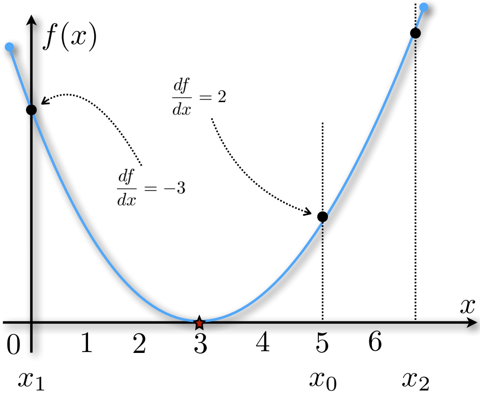
...

x_t converges **very slowly**.

Effect of very large step-size α...

$$\min_{x \in \mathbb{R}} \frac{1}{2}(x-3)^2$$

$$\frac{df}{dx} = x - 3$$



Choose $x_0 = 5$ and $\boldsymbol{\alpha = \frac{5}{2}}$

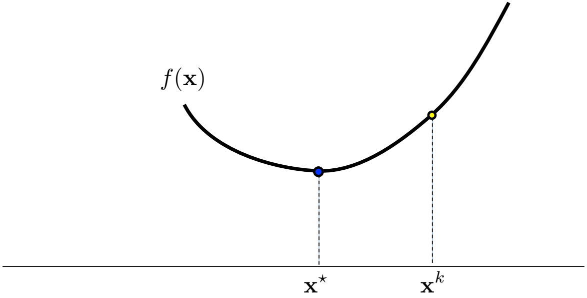
$x_1 = x_0 - \alpha \frac{df}{dx}\Big|_{x=x_0} = 5 - \frac{5}{2}2 = 0$

$x_2 = x_1 - \alpha \frac{df}{dx}\Big|_{x=x_1} = 0 - \frac{5}{2}(-3) = \frac{15}{2}$

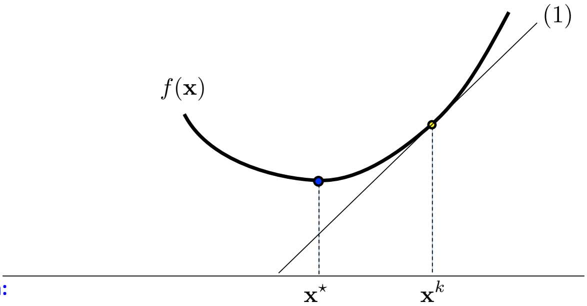
...

x_t **diverges**.

A geometrical intuition: How does smoothness help?



A geometrical intuition: How does smoothness help?



Structure in optimization:

$$(1) \qquad f(\mathbf{x}) \geq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle$$

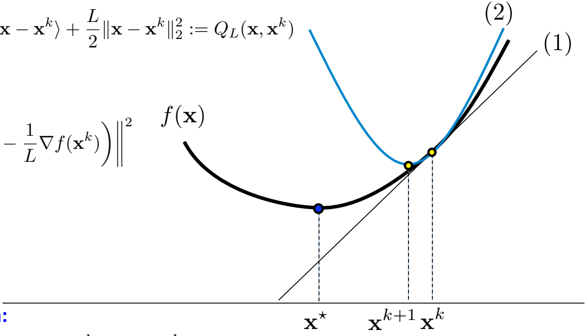
A geometrical intuition: How does smoothness help?

Majorize:

$$f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2 := Q_L(\mathbf{x}, \mathbf{x}^k)$$

Minimize:

$$\begin{aligned}\mathbf{x}^{k+1} &= \arg\min_{\mathbf{x}} Q_L(\mathbf{x}, \mathbf{x}^k) \\ &= \arg\min_{\mathbf{x}} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k) \right) \right\|^2 \\ &= \mathbf{x}^k - \frac{1}{L}\nabla f(\mathbf{x}^k)\end{aligned}$$



Structure in optimization:

(1) $\quad f(\mathbf{x}) \geq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle$

(2) $\quad f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

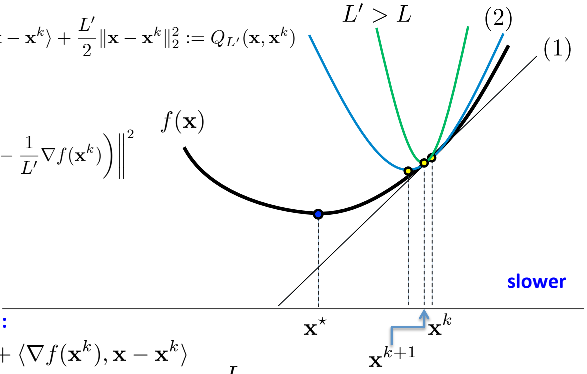
A geometrical intuition: How does smoothness help?

Majorize:

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

Minimize:

$$\begin{aligned}\mathbf{x}^{k+1} &= \arg\min_{\mathbf{x}} Q_{L'}(\mathbf{x}, \mathbf{x}^k) \\ &= \arg\min_{\mathbf{x}} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L'}\nabla f(\mathbf{x}^k) \right) \right\|^2 \\ &= \mathbf{x}^k - \frac{1}{L'}\nabla f(\mathbf{x}^k)\end{aligned}$$

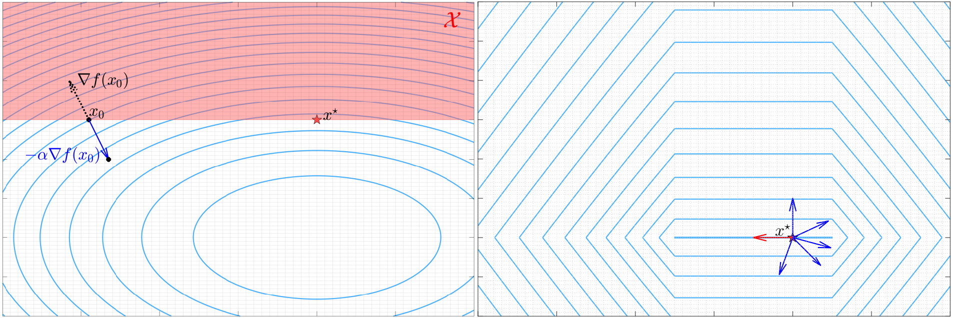


Structure in optimization:

(1) $\quad f(\mathbf{x}) \geq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle$

(2) $\quad f(\mathbf{x}) \leq f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{L}{2}\|\mathbf{x} - \mathbf{x}^k\|_2^2$

Stationarity measures with constraints & non-smoothness



- Smooth: Gradient mapping norm
  - $\|G_\alpha(x_t)\|^2 = \frac{1}{\alpha^2}\|x_t - P_{\mathcal{X}}(x_t - \alpha\nabla f(x_t))\|^2$
  - $P_{\mathcal{X}}$ denotes the projection operator to $\mathcal{X}$
  - possible to compute
- Non-smooth: Generalized subdifferential distance
  - $\text{dist}(0, \partial(f(x_t) + \delta_{\mathcal{X}}(x_t)))^2$
  - $\delta_{\mathcal{X}}$ refers to the indicator function for the set $\mathcal{X}$
  - hard in general (even approximately)

The one formula is very flexible

$$\Phi^\star = \min_{x:x\in\mathcal{X}} \max_{y:y\in\mathcal{Y}} \Phi(x,y) \quad (\operatorname{argmin}\operatorname{argmax} \rightarrow x^\star, y^\star)$$

The one formula is very flexible

$$\Phi^\star = \min_{x:x\in\mathcal{X}} \underbrace{\max_{y:y\in\mathcal{Y}} \Phi(x,y)}_{f(x)} \quad (\text{argmin argmax} \to x^\star, y^\star)$$

$$f^\star = \min_{x:x\in\mathcal{X}} f(x) \quad (\text{argmin} \to x^\star)$$

Application: Adversarial training

Figure: (Left) An ℓ_∞-attack: The alteration is hard to perceive. (Right) An ℓ_1-attack: The alteration in this case is obvious.

Adversarial Training

Let $h_x : \mathbb{R}^n \to \mathbb{R}$ be a model with parameters x and let $\{(\mathbf{a}_i, b_i)\}_{i=1}^n$, with the data $\mathbf{a}_i \in \mathbb{R}^p$ and the labels $\mathbf{b}_i$. The problem of adversarial training is the following adversarial optimization problem

$$\min_x \frac{1}{n} \sum_{i=1}^n \left[\max_{\eta : \|\eta\| \le \epsilon} L(h_x(\mathbf{a}_i + \eta), b_i) \right] \approx \min_x \mathbb{E}_{(\mathbf{a},b)\sim\mathbb{P}} \left[\max_{\eta : \|\eta\| \le \epsilon} L(h_x(\mathbf{a}_i + \eta), b_i) \right].$$

Note the similarity with the template $\min_{x\in\mathcal{X}} \max_{y\in\mathcal{Y}} \Phi(x, y)$.

Danskin's theorem

Danskin's theorem (Bertsekas variant)

Let $\Phi(x, y) : \mathbb{R}^p \times \mathcal{Y} \to \mathbb{R}$, where $\mathcal{Y} \subset \mathbb{R}^m$ is a compact set and define $f(x) := \max_{y \in \mathcal{Y}} \Phi(x, y)$. Let $\Phi(x, y)$ is an extended real-valued closed proper convex function for each y in the compact set $\mathcal{Y}$; the interior of the domain of f is nonempty; $\Phi(x, y)$ is jointly continuous on the relative interior of the domain of f and $\mathcal{Y}$.

Define $\mathcal{Y}^\star := \arg\max_{y \in \mathcal{Y}} \Phi(x, y)$ as the set of maximizers and $y^\star \in \mathcal{Y}^\star$ as an element of this set. We have

1. $f(x)$ is a convex function.
2. If $y^\star = \arg\max_{y \in \mathcal{Y}} \Phi(x, y)$ is unique, then the function $f(x) = \max_{y \in \mathcal{Y}} \Phi(x, y)$ is differentiable at x:

$$\nabla_x f(x) = \nabla_x \left(\max_{y \in \mathcal{Y}} \phi(x, y) \right) = \nabla_x \Phi(x, y^\star).$$

3. If $y^\star = \arg\max_{y \in \mathcal{Y}} \Phi(x, y)$ is not unique, then the subdifferential $\partial_x f(x)$ of f is given by

$$\partial_x f(x) = \text{conv} \left\{ \partial_x \Phi(x, y^\star) : y^\star \in \mathcal{Y}^\star \right\}.$$

Remarks:

- The adversarial problem is not convex in x in general.
- With proper initialization, overparameterization works argue that it is effectively convex.
- (Sub)Gradients of f_i are calculated as $\partial f_i(x) = \nabla_x L(h_x(\mathbf{a}_i + \eta^\star(x)), b_i)$.

A corollary to Danskin's theorem

Adversarial Training

Let $h_x : \mathbb{R}^n \to \mathbb{R}$ be a model with parameters x and let $\{(\mathbf{a}_i, b_i)\}_{i=1}^n$, with $\mathbf{a}_i \in \mathbb{R}^p$ and b_i be the corresponding labels. The adversarial training optimization problem is given by

$$\min_x \left\{ \frac{1}{n}\sum_{i=1}^n f_i(x) := \frac{1}{n}\sum_{i=1}^n \underbrace{\left[\max_{\eta:\|\eta\|_\infty \le \epsilon} L(h_x(\mathbf{a}_i + \eta), b_i) \right]}_{=: f_i(x)} \right\}.$$

L is not continuously differentiable due to ReLU, max-pooling, etc.

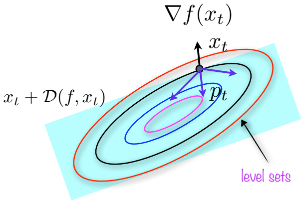


Figure: Descent directions in 2D should be an element of the cone of descent directions $\mathcal{D}(f, \cdot)$.

Descent directions [4]

Define $\mathcal{Y}^\star := \arg\max_{y\in\mathcal{Y}} \Phi(x, y)$ as the set of maximizers, $y^\star \in \mathcal{Y}^\star$, and $f(x) := \max_{y\in\mathcal{Y}} \Phi(x, y)$. As long as $\nabla_x \Phi(x, y^\star)$ is non-zero, it is a descent direction (and not a subgradient!) for $f(x)$.

Remarks:

- $\nabla_x L(h_x(\mathbf{a}_i + \eta^\star(x)), b_i)$ is a descent direction for $f_i(x)$.
- We cannot find global maximizers $\mathcal{Y}^\star$.
- Only when $y^\star$ is a singleton, $\nabla_x L(h_x(\mathbf{a}_i + \eta^\star(x)), b_i)$ is a (sub)gradient [1].

A more general minimax problem: Generative adversarial networks

Vanilla GAN [2]

$$\min_{x \in \mathcal{X}} \max_{y \in \mathcal{Y}} \mathbb{E}_{\mathbf{a} \sim \hat{\mu}_n} [\log \mathbf{d}_y(\mathbf{a})] + \mathbb{E}_{\boldsymbol{\omega} \sim \mathrm{p}_\Omega} [\log (1 - \mathbf{d}_y(h_x(\boldsymbol{\omega})))] \tag{1}$$

- Binary cross-entropy modeling.
- $\mathbf{d}_y(\mathbf{a}) : \mathcal{Y} \to [0,1]$ represents the probability that $\mathbf{a}$ came from the real data distribution $\mu^\natural$.

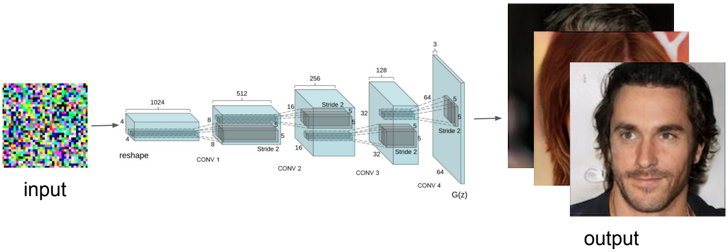


Figure: Schematic of a generative model, $h_x(\boldsymbol{\omega})$ [2, 3].

Worst-case iteration complexities of classical projected first-order methods[1,2]

$f(x)$	gradient oracle	L-smooth	Stationarity measure	**GD/SGD**	**Accelerated GD/SGD**
Convex	stochastic	yes	$f(x_t) - f^\star =$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$
Convex	deterministic	yes	$f(x_t) - f^\star =$	$\mathcal{O}\left(\frac{1}{t}\right)$	$\mathcal{O}\left(\frac{1}{t^2}\right)$
Convex	stochastic	no	$f(x_t) - f^\star =$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$
Nonconvex	stochastic	yes	$\|G_\eta(x_t)\|^2 =$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$[3]	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$[3]
Nonconvex	deterministic	yes	$\|G_\eta(x_t)\|^2 =$	$\mathcal{O}\left(\frac{1}{t}\right)$[4]	$\mathcal{O}\left(\frac{1}{t}\right)$[4]
Nonconvex	stochastic	no	$\text{dist}(0, \partial(f(x_t) + \delta_{\mathcal{X}}(x_t)))^2 =$	?[3,5,6]	?[3,5,6]

- Basic structures, such as smoothness or strong convexity, help, but there are more structures that can be used:
  - $\max$-form, metric subregularity, Polyak-Lojasiewicz, Kurdyka-Lojasiewicz, weak convexity,[3] growth cond...

[1] Y. Nesterov, "Introductory lectures on convex optimization: A basic course," Springer Science, 2013.

[2] Y. Carmon, J.C. Duchi, O. Hinder, and A. Sidford, "Lower bounds for finding stationary points I–II." Mathematical Programming, 2019.

[3] D. Davis and D. Drusvyatskiy, "Stochastic model-based minimization of weakly convex functions," SIOPT, 2019.

[4] S. Ghadimi and G. Lan, "Accelerated gradient methods for nonconvex nonlinear and stochastic programming," MathProg, 2016.

[5] J. Zhang, et al., "On complexity of finding stationary points of nonsmooth nonconvex functions," arXiv:2002.04130, 2020.

[6] O. Shamir, "Can We Find Near-Approximately-Stationary Points of Nonsmooth Nonconvex Functions?" arXiv:2002.11962, 2020.

Worst-case iteration complexities of classical projected first-order methods[1,2]

$f(x)$	gradient oracle	L-smooth	Stationarity measure	GD/SGD	Accelerated GD/SGD
Convex	stochastic	yes	$f(x_t) - f^\star =$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$
Convex	deterministic	yes	$f(x_t) - f^\star =$	$\mathcal{O}\left(\frac{1}{t}\right)$	$\mathcal{O}\left(\frac{1}{t^2}\right)$
Convex	stochastic	no	$f(x_t) - f^\star =$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)$
Nonconvex	stochastic	yes	$\|G_\eta(x_t)\|^2 =$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)^3$	$\mathcal{O}\left(\frac{1}{\sqrt{t}}\right)^3$
Nonconvex	deterministic	yes	$\|G_\eta(x_t)\|^2 =$	$\mathcal{O}\left(\frac{1}{t}\right)^4$	$\mathcal{O}\left(\frac{1}{t}\right)^4$
Nonconvex	stochastic	no	$\mathrm{dist}(0, \partial(f(x_t) + \delta_{\mathcal{X}}(x_t)))^2 =$	?[3,5,6]	?[3,5,6]

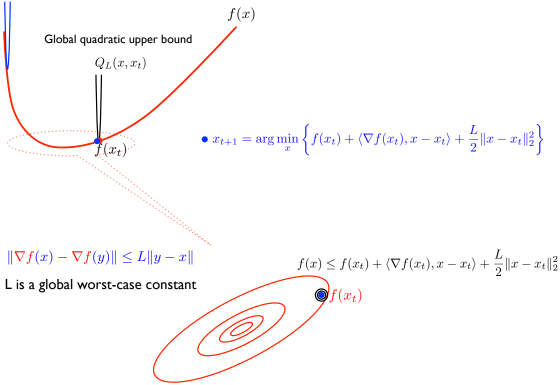
at the end of the presentation

- Basic structures, such as smoothness or strong convexity, help, but there are more structures that can be used:
  - $\max$-form, metric subregularity, Polyak-Lojasiewicz, Kurdyka-Lojasiewicz, weak convexity,[3] growth cond...

[1] Y. Nesterov, "Introductory lectures on convex optimization: A basic course," Springer Science, 2013.
[2] Y. Carmon, J.C. Duchi, O. Hinder, and A. Sidford, "Lower bounds for finding stationary points I–II." Mathematical Programming, 2019.
[3] D. Davis and D. Drusvyatskiy, "Stochastic model-based minimization of weakly convex functions," SIOPT, 2019.
[4] S. Ghadimi and G. Lan, "Accelerated gradient methods for nonconvex nonlinear and stochastic programming," MathProg, 2016.
[5] J. Zhang, et al., "On complexity of finding stationary points of nonsmooth nonconvex functions," arXiv:2002.04130, 2020.
[6] O. Shamir, "Can We Find Near-Approximately-Stationary Points of Nonsmooth Nonconvex Functions?" arXiv:2002.11962, 2020.

Worst-case is often too pessimistic

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



- Rates are not everything!
  - overall computational effort is what matters
  - constants &implementations are key
- Knowledge of smoothness, the value of L,...
  - challenging
- Must "somehow" adapt to a "different" function
  - online and without knowing L
  - can reduce overall computational effort!

References I

[1] Dimitris Bertsimas, Omid Nohadani, and Kwong Meng Teo.
Robust nonconvex optimization for simulation-based problems.
Operations Research, 2007.

[2] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio.
Generative adversarial nets.
In Z. Ghahramani, M. Welling, C. Cortes, N. D. Lawrence, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems 27*, pages 2672–2680. Curran Associates, Inc., 2014.

[3] Tero Karras, Timo Aila, Samuli Laine, and Jaakko Lehtinen.
Progressive growing of GANs for improved quality, stability, and variation.
In *International Conference on Learning Representations*, 2018.

[4] Aleksander Madry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, and Adrian Vladu.
Towards deep learning models resistant to adversarial attacks.
In *International Conference on Learning Representations*, 2018.