Mathematics of Data: From Theory to Computation

Prof Volkan Cevher volkan.cevher@epfl.ch

Lecture 3: Unconstrained, smooth minimization I

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

EE-556 (Fall 2019)













License Information for Mathematics of Data Slides

► This work is released under a <u>Creative Commons License</u> with the following terms:

Attribution

▶ The licensor permits others to copy, distribute, display, and perform the work. In return, licensees must give the original authors credit.

Non-Commercial

 The licensor permits others to copy, distribute, display, and perform the work. In return, licensees may not use the work for commercial purposes – unless they get the licensor's permission.

Share Alike

- ► The licensor permits others to distribute derivative works only under a license identical to the one that governs the licensor's work.
- ► Full Text of the License

Outline

- ► This lecture
 - 1. Unconstrained convex & non-convex optimization: the basics
 - 2. Gradient descent methods
- Next lecture
 - 1. Gradient and accelerated gradient descent methods

Recommended reading

- Chapters 2, 3, 5, 6 in Nocedal, Jorge, and Wright, Stephen J., Numerical Optimization, Springer, 2006.
- Chapter 9 in Boyd, Stephen, and Vandenberghe, Lieven, Convex optimization, Cambridge university press, 2009.
- Chapter 1 in Bertsekas, Dimitris, Nonlinear Programming, Athena Scientific, 1999.
- Chapters 1, 2 and 4 in Nesterov, Yurii, Introductory Lectures on Convex Optimization: A Basic Course, Vol. 87, Springer, 2004.

Motivation

Motivation

This lecture covers the basics of numerical methods for *unconstrained* and *smooth* minimization for **convex** and **non-convex** problem settings in a unified manner.

Smooth unconstrained convex minimization

Problem (Mathematical formulation)

The unconstrained convex minimization problem is defined as:

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

- f is a proper, closed and smooth convex function, $-\infty < f^* < +\infty$.
- ▶ The solution set $S^* := \{ \mathbf{x}^* \in \text{dom}(f) : f(\mathbf{x}^*) = f^* \}$ is nonempty.

Example: Maximum likelihood estimation and M-estimators

Problem

Let $\mathbf{x}^{\natural} \in \mathbb{R}^p$ be unknown and $b_1, ..., b_n$ be i.i.d. samples of a random variable B with p.d.f. $p_{\mathbf{x}^{\natural}}(b) \in \mathcal{P} := \{p_{\mathbf{x}}(b) : \mathbf{x} \in \mathbb{R}^p\}$. Goal: Estimate \mathbf{x}^{\natural} from $b_1, ..., b_n$.

Optimization formulation (ML estimator)

$$\hat{\mathbf{x}}_{\mathsf{ML}} := \arg\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ -\frac{1}{n} \sum_{i=1}^n \ln\left[p_{\mathbf{x}}(b_i)\right] \right\} = \arg\min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x})$$

Theorem (Performance of the ML estimator [2, 5])

The random variable $\hat{\mathbf{x}}_{MI}$ satisfies

$$\lim_{n \to \infty} \sqrt{n} \mathbf{J}^{-1/2} \left(\hat{\mathbf{x}}_{ML} - \mathbf{x}^{\natural} \right) \stackrel{d}{=} Z \sim \mathcal{N}(\mathbf{0}, \mathbf{I}),$$

where

$$\mathbf{J} := -\mathbb{E}\left[\nabla_{\mathbf{x}}^2 \ln\left[p_{\mathbf{x}}(B)\right]\right]\Big|_{\mathbf{x} = \mathbf{x}^{\natural}}.$$

is the Fisher information matrix associated with one sample. Roughly speaking,

$$\left\| \sqrt{n} \, \mathbf{J}^{-1/2} \left(\hat{\mathbf{x}}_{\mathit{ML}} - \mathbf{x}^{\natural} \right) \right\|_{2}^{2} \sim \mathrm{Tr} \left(\mathbf{I} \right) = p \quad \Rightarrow \qquad \boxed{ \left\| \hat{\mathbf{x}}_{\mathit{ML}} - \mathbf{x}^{\natural} \right\|_{2}^{2} = \mathcal{O}(p/n) } \, .$$

Example: Maximum likelihood estimation and M-estimators

Problem

Let $\mathbf{x}^{\natural} \in \mathbb{R}^p$ be unknown and $b_1,...,b_n$ be i.i.d. samples of a random variable B with p.d.f. $p_{\mathbf{x}^{\natural}}(b) \in \mathcal{P} := \{p_{\mathbf{x}}(b) : \mathbf{x} \in \mathbb{R}^p\}$. Goal: Estimate \mathbf{x}^{\natural} from b_1,\ldots,b_n .

Optimization formulation (ML estimator)

$$\hat{\mathbf{x}}_{\mathsf{ML}} := \arg\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ -\frac{1}{n} \sum_{i=1}^n \ln\left[p_{\mathbf{x}}(b_i)\right] \right\} = \arg\min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x})$$

Optimization formulation (M-estimator)

In general, we can replace the negative log-likelihoods by any appropriate, convex g_i 's

$$\min_{x \in \mathcal{X}} \frac{1}{n} \sum_{i=1}^{n} g_i(b_i; \mathbf{x}).$$

Approximate vs. exact optimality

Is it possible to solve a convex optimization problem?

"In general, optimization problems are unsolvable" - Y. Nesterov [3]

- ▶ Even when a closed-form solution exists, numerical accuracy may still be an issue.
- ▶ We must be content with approximately optimal solutions.

Definition

We say that $\mathbf{x}^{\star}_{\epsilon}$ is ϵ -optimal in **objective value** if

$$f(\mathbf{x}_{\epsilon}^{\star}) - f^{\star} \le \epsilon$$
.

Definition

We say that $\mathbf{x}^\star_\epsilon$ is ϵ -optimal in **sequence** if, for some norm $\|\cdot\|$,

$$\|\mathbf{x}_{\epsilon}^{\star} - \mathbf{x}^{\star}\| \leq \epsilon$$
,

► The latter approximation guarantee is considered stronger.

A gradient method

Lemma (First-order necessary optimality condition)

Let x^* be a global minimum of a differentiable convex function f. Then, it holds that

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

Fixed-point characterization

Multiply by -1 and add x^* to both sides to obtain a fixed point condition,

$$\mathbf{x}^{\star} = \mathbf{x}^{\star} - \alpha \nabla f(\mathbf{x}^{\star}) \qquad \text{for all } 0 \neq \alpha \in \mathbb{R}$$

Gradient method

Choose a starting point x^0 and iterate

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

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

When does the gradient method converge?

Lemma

Let f be a closed, convex function. Assume that

- 1. There exists $\mathbf{x}^* \in \text{dom}(f)$ such that $\nabla f(\mathbf{x}^*) = 0$.
- 2. The mapping $\psi(\mathbf{x}) = \mathbf{x} \alpha \nabla f(\mathbf{x})$ is contractive for some α : i.e., there exists $\gamma \in [0,1)$ such that

$$\|\psi(\mathbf{x}) - \psi(\mathbf{z})\| \leq \gamma \|\mathbf{x} - \mathbf{z}\| \quad \textit{for all } \mathbf{x}, \mathbf{z} \in \text{dom}(f)$$

Then, for any starting point $\mathbf{x}^0 \in \text{dom}(f)$, the gradient method converges to \mathbf{x}^* .

When does the gradient method converge?

Lemma

Let f be a closed, convex function. Assume that

- 1. There exists $\mathbf{x}^* \in \text{dom}(f)$ such that $\nabla f(\mathbf{x}^*) = 0$.
- 2. The mapping $\psi(\mathbf{x}) = \mathbf{x} \alpha \nabla f(\mathbf{x})$ is contractive for some α : i.e., there exists $\gamma \in [0,1)$ such that

$$\|\psi(\mathbf{x}) - \psi(\mathbf{z})\| \le \gamma \|\mathbf{x} - \mathbf{z}\| \quad \textit{for all } \mathbf{x}, \mathbf{z} \in \text{dom}(f)$$

Then, for any starting point $\mathbf{x}^0 \in \text{dom}(f)$, the gradient method converges to \mathbf{x}^* .

Proof.

If we start the gradient method at $\mathbf{x}^0 \in \text{dom}(f)$, then we have

$$\begin{split} \|\mathbf{x}^{k+1} - \mathbf{x}^{\star}\| &= \|\mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k) - \mathbf{x}^{\star}\| \\ &= \|\psi(\mathbf{x}^k) - \psi(\mathbf{x}^{\star})\| \qquad \qquad \text{(fixed-point characterization)} \\ &\leq \gamma \|\mathbf{x}^k - \mathbf{x}^{\star}\| \qquad \qquad \text{(contractiveness)} \\ &< \gamma^{k+1} \|\mathbf{x}^0 - \mathbf{x}^{\star}\| \; . \end{split}$$

We then have that the sequence $\{x^k\}$ converges globally to x^* at a linear rate.

Short (but important) detour: convergence rates

Definition (Convergence of a sequence)

The sequence $\mathbf{u}^1, \mathbf{u}^2, ..., \mathbf{u}^k, ...$ converges to \mathbf{u}^* (denoted $\lim_{k \to \infty} \mathbf{u}^k = \mathbf{u}^*$), if

$$\forall \ \varepsilon > 0, \exists \ K \in \mathbb{N} : k \ge K \Rightarrow \|\mathbf{u}^k - \mathbf{u}^\star\| \le \varepsilon$$

Convergence rates: the "speed" at which a sequence converges

sublinear: if there exists c > 0 such that

$$\|\mathbf{u}^k - \mathbf{u}^\star\| = O(k^{-c})$$

▶ linear: if there exists $\alpha \in (0,1)$ such that

$$\|\mathbf{u}^k - \mathbf{u}^\star\| = O(\alpha^k)$$

Q-linear: if there exists a constant $r \in (0,1)$ such that

$$\lim_{k \to \infty} \frac{\|\mathbf{u}^{k+1} - \mathbf{u}^{\star}\|}{\|\mathbf{u}^k - \mathbf{u}^{\star}\|} = r$$

- superlinear: If r = 0, we say that the sequence converges superlinearly.
- **quadratic:** if there exists a constant $\mu > 0$ such that

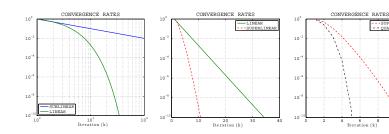
$$\lim_{k \to \infty} \frac{\|\mathbf{u}^{k+1} - \mathbf{u}^{\star}\|}{\|\mathbf{u}^{k} - \mathbf{u}^{\star}\|^{2}} = \mu$$

Example: Convergence rates

Examples of sequences that all converge to $u^* = 0$:

- Sublinear: $u^k = 1/k$
- ▶ Linear: $u^k = 0.5^k$

- ▶ Superlinear: $u^k = k^{-k}$
- Quadratic: $u^k = 0.5^{2^k}$



Remark

For **unconstrained** convex minimization as in (1), we always have $f(\mathbf{x}^k) - f^* \ge 0$. Hence, we do not need to use the absolute value when we show convergence results based on the objective value, such as $f(\mathbf{x}^k) - f^* \le O(1/k^2)$, which is sublinear.

Contractive maps and convexity

Proposition (Contractivity implies convexity with structure)

Let $f \in \mathcal{C}^2$ and define $\psi(\mathbf{x}) = \mathbf{x} - \alpha \nabla f(\mathbf{x})$, with $\alpha > 0$. If $\psi(\mathbf{x})$ is contractive, with a constant contraction factor $\gamma < 1$, then $f \in \mathcal{F}^{2,1}_{L,n}$.

Proof.

Consider $\mathbf{y} = \mathbf{x} + t\Delta \mathbf{x}$. By the contractivity assumption it must hold that

$$\|\psi(\mathbf{x} + t\Delta\mathbf{x}) - \psi(\mathbf{x})\| \le t\gamma \|\Delta\mathbf{x}\| \quad \forall t.$$

We also have that

$$\lim_{t \to 0} \frac{1}{t} \| \psi(\mathbf{x} + t\Delta \mathbf{x}) - \psi(\mathbf{x}) \| = \lim_{t \to 0} \| \Delta \mathbf{x} - \frac{\alpha}{t} \left(\nabla f(\mathbf{x} + t\Delta \mathbf{x}) - \nabla f(\mathbf{x}) \right) \|$$

$$= \| \left(\mathbf{I} - \alpha \nabla^2 f(\mathbf{x}) \right) \Delta \mathbf{x} \|$$

$$\leq \gamma \| \Delta \mathbf{x} \| \qquad \text{(by assumption)}$$

The inequality implies (derivation on the board) that

$$\mathbf{0} \prec \frac{1-\gamma}{\alpha} \mathbf{I} \preceq \nabla^2 f(\mathbf{x}) \preceq \frac{1+\gamma}{\alpha} \mathbf{I},$$

which can be reinterpreted as $f \in \mathcal{F}_{L,\mu}^{2,1}$ with $L = \frac{1+\gamma}{\alpha}$ and $\mu = \frac{1-\gamma}{\alpha}$ (next!).



Gradient descent methods

Definition

Gradient descent (GD) Starting from $\mathbf{x}^0 \in \mathrm{dom}(f)$, update $\{\mathbf{x}^k\}_{k \geq 0}$ as

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

Notice that $\mathbf{p}^k := -\nabla f(\mathbf{x}^k)$ is the steepest descent (anti-gradient) search direction.

Key question: how to choose α_k to have descent/contraction?

Gradient descent methods

Definition

Gradient descent (GD) Starting from $\mathbf{x}^0 \in \mathrm{dom}(f)$, update $\{\mathbf{x}^k\}_{k \geq 0}$ as

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

Notice that $\mathbf{p}^k := -\nabla f(\mathbf{x}^k)$ is the steepest descent (anti-gradient) search direction.

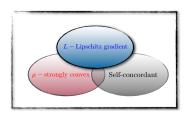
Key question: how to choose α_k to have descent/contraction?

We need structure!

We use \mathcal{F} to denote the class of smooth convex functions.

(The domain of each function will be apparent from the context.)

Next few slides: structural assumptions



L-Lipschitz gradient class of functions

Definition (*L*-Lipschitz gradient convex functions)

Let $f:\mathcal{Q}\to\mathbb{R}$ be differentiable and convex, i.e., $f\in\mathcal{F}^1(\mathcal{Q})$. Then, f has a Lipschitz gradient if there exists L>0 (the Lipschitz constant) s.t.

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \le L\|\mathbf{x} - \mathbf{y}\|_2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{Q}.$$

Proposition (*L*-Lipschitz gradient convex functions)

 $f \in \mathcal{F}^1(\mathcal{Q})$ has L-Lipschitz gradient if and only if the following function is convex:

$$h(\mathbf{x}) = \frac{L}{2} \|\mathbf{x}\|_2^2 - f(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{Q}.$$

Definition (Class of 2-nd order Lipschitz functions)

The class of twice continuously differentiable functions f on $\mathcal Q$ with Lipschitz continuous Hessian is denoted as $\mathcal F_t^{2,2}(\mathcal Q)$ (with $2\to 2$ denoting the spectral norm)

$$\|\nabla^2 f(\mathbf{x}) - \nabla^2 f(\mathbf{y})\|_{2\to 2} \le L\|\mathbf{x} - \mathbf{y}\|_2, \quad \forall \mathbf{x}, \mathbf{y} \in Q,$$

 $ightharpoonup \mathcal{F}_L^{l,m}$: functions that are l-times differentiable with m-th order Lipschitz property.



Example: Logistic regression

Problem (Logistic regression)

Given a sample vector $\mathbf{a}_i \in \mathbb{R}^p$ and a binary class label $b_i \in \{-1, +1\}$ (i = 1, ..., n), we define the conditional probability of b_i given \mathbf{a}_i as:

$$\mathbb{P}(b_i|\mathbf{a}_i,\mathbf{x}^{\natural},\mu) \propto 1/(1+e^{-b_i(\langle\mathbf{x}^{\natural},\mathbf{a}_i\rangle+\mu)}),$$

where $\mathbf{x}^{\natural} \in \mathbb{R}^p$ is some true weight vector, $\mu \in \mathbb{R}$ is called the intercept. How to estimate \mathbf{x}^{\natural} given the sample vectors, the binary labels, and μ ?

Optimization formulation

$$\min_{\mathbf{x} \in \mathbb{R}^p} \underbrace{\frac{1}{n} \sum_{i=1}^n \log(1 + \exp(-b_i(\mathbf{a}_i^T \mathbf{x} + \mu)))}_{f(\mathbf{x})}$$

Structural properties

Let $\mathbf{A} = [\mathbf{a}_1, \dots, \mathbf{a}_n]^T$ (design matrix), then $f \in \mathcal{F}_L^{2,1}$, with $L = \frac{1}{4} \|\mathbf{A}^T \mathbf{A}\|$

μ -strongly convex functions

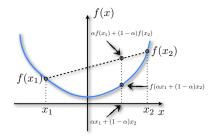
Definition

A function $f:\mathcal{Q}\to\mathbb{R}\cup\{+\infty\}$, $\mathcal{Q}\subseteq\mathbb{R}^p$ is called μ -strongly convex on its domain if and only if for any $\mathbf{x},\ \mathbf{y}\in\mathcal{Q}$ and $\alpha\in[0,1]$ we have:

$$f(\alpha \mathbf{x} + (1 - \alpha)\mathbf{y}) \le \alpha f(\mathbf{x}) + (1 - \alpha)f(\mathbf{y}) - \frac{\mu}{2}\alpha(1 - \alpha)\|\mathbf{x} - \mathbf{y}\|_2^2.$$

The constant μ is called the convexity parameter of function f.

- ▶ The class of k-differentiable μ -strongly functions is denoted as $\mathcal{F}^k_{\mu}(\mathcal{Q})$.
- ► Strong convexity ⇒ strict convexity, BUT strict convexity ⇒ strong convexity





lions@epfl

Alternative: μ -strongly convex functions

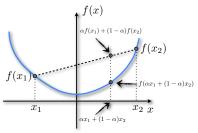
Definition

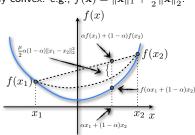
A convex function $f:\mathcal{Q} \to \mathbb{R}$ is said to be $\mu\text{-strongly convex}$ if

$$h(\mathbf{x}) = f(\mathbf{x}) - \frac{\mu}{2} ||\mathbf{x}||_2^2$$

is convex, where μ is called the strong convexity parameter.

- ▶ The class of k-differentiable μ -strongly functions is denoted as $\mathcal{F}^k_{\mu}(\mathcal{Q})$.
- Non-smooth functions can be μ -strongly convex: e.g., $f(\mathbf{x}) = \|\mathbf{x}\|_1 + \frac{\mu}{2} \|\mathbf{x}\|_2^2$.





Example: Least-squares estimation

Problem

Let $\mathbf{x}^{\natural} \in \mathbb{R}^p$ and $\mathbf{A} \in \mathbb{R}^{n \times p}$ (full column rank). Goal: estimate \mathbf{x}^{\natural} , given \mathbf{A} and

$$\mathbf{b} = \mathbf{A}\mathbf{x}^{\natural} + \mathbf{w},$$

where w denotes unknown noise.

Optimization formulation (Least-squares estimator)

$$\min_{\mathbf{x} \in \mathbb{R}^p} \frac{1}{2} \frac{\|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2}{f(\mathbf{x})}.$$

Structural properties

- $ightharpoonup
 abla f(\mathbf{x}) = \mathbf{A}^T (\mathbf{A}\mathbf{x} \mathbf{b}), \text{ and }
 abla^2 f(\mathbf{x}) = \mathbf{A}^T \mathbf{A}.$
- lacksquare $\lambda_p \mathbf{I} \preceq \nabla^2 f(\mathbf{x}) \preceq \lambda_1 \mathbf{I}$, where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p$ are the eigenvalues of $\mathbf{A}^T \mathbf{A}$.
- It follows that $L=\lambda_1$ and $\mu=\lambda_p$. If $\lambda_p>0$, then $f\in\mathcal{F}^{2,1}_{L,\mu}$, otherwise $f\in\mathcal{F}^{2,1}_{L}$.
- ▶ Since rank($\mathbf{A}^T \mathbf{A}$) $\leq \min\{n, p\}$, if n < p, then $\lambda_p = 0$.

*Self-concordant functions

Definition (Self-concordant functions in 1-dimension)

A convex function $\varphi:\mathbb{R}\to\mathbb{R}$ is self-concordant if

$$|\varphi'''(t)| \le 2\varphi''(t)^{3/2}, \quad \forall t \in \mathbb{R}.$$

*Self-concordant functions

Definition (Self-concordant functions in 1-dimension)

A convex function $\varphi:\mathbb{R}\to\mathbb{R}$ is self-concordant if

$$|\varphi'''(t)| \le 2\varphi''(t)^{3/2}, \quad \forall t \in \mathbb{R}.$$

Affine Invariance of self-concordant functions

Let $\tilde{\varphi}(t) = \varphi(\alpha t + \beta)$ where $\alpha \neq 0$. Then, $\tilde{\varphi}$ is self-concordant iff φ is.

*Self-concordant functions

Definition (Self-concordant functions in 1-dimension)

A convex function $\varphi:\mathbb{R}\to\mathbb{R}$ is self-concordant if

$$|\varphi'''(t)| \le 2\varphi''(t)^{3/2}, \quad \forall t \in \mathbb{R}.$$

Affine Invariance of self-concordant functions

Let $\tilde{\varphi}(t) = \varphi(\alpha t + \beta)$ where $\alpha \neq 0$. Then, $\tilde{\varphi}$ is self-concordant iff φ is.

Important remarks of self-concordance

- 1. Generalize to higher dimension: A convex function $f: \mathbb{R}^n \to \mathbb{R}$ is said to be (standard) self-concordant if $|\varphi'''(t)| \leq 2\varphi''(t)^{3/2}$, where $\varphi(t) := f(\mathbf{x} + t\mathbf{v})$ for all $t \in \mathbb{R}$, $\mathbf{x} \in \mathrm{dom}\, f$ and $\mathbf{v} \in \mathbb{R}^n$ such that $\mathbf{x} + t\mathbf{v} \in \mathrm{dom}\, f$.
- 2. Affine invariance still holds in high dimension.
- 3. Self-concordant functions are efficiently minimized by the Newton method and its variants (see Lecture 6).

Back to gradient descent methods

Gradient descent (GD) algorithm

Starting from $\mathbf{x}^0 \in \mathrm{dom}(f)$, produce the sequence $\mathbf{x}^1,...,\mathbf{x}^k,...$ according to

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

Notice that $\mathbf{p}^k := -\nabla f(\mathbf{x}^k)$ is the steepest descent (anti-gradient) direction. **Key question**: how do we choose α_k to have descent/contraction?

Back to gradient descent methods

Gradient descent (GD) algorithm

Starting from $\mathbf{x}^0 \in \mathrm{dom}(f)$, produce the sequence $\mathbf{x}^1,...,\mathbf{x}^k,...$ according to

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

Notice that $\mathbf{p}^k := -\nabla f(\mathbf{x}^k)$ is the steepest descent (anti-gradient) direction. **Key question**: how do we choose α_k to have descent/contraction?

Step-size selection

Case 1: If $f \in \mathcal{F}_L^{1,1}(\mathbb{R}^p)$, then:

- $lackbox{ We can choose } 0<lpha_k<rac{2}{L}.$ The optimal choice is $lpha_k:=rac{1}{L}.$
- $ightharpoonup \alpha_k$ can be determined by a line-search procedure:
 - 1. Exact line search: $\alpha_k := \arg\min_{\alpha > 0} f(\mathbf{x}^k \alpha \nabla f(\mathbf{x}^k))$.
 - 2. Back-tracking line search with Armijo-Goldstein's condition:

$$f(\mathbf{x}^k - \alpha \nabla f(\mathbf{x}^k)) \le f(\mathbf{x}^k) - c\alpha \|\nabla f(\mathbf{x}^k)\|^2, \ c \in (0, 1/2].$$

Case 2: If $f \in \mathcal{F}_{L,\mu}^{1,1}(\mathbb{R}^p)$, then:

 $lackbox{ We can choose } 0<lpha_k\leq rac{2}{L+\mu}.$ The optimal choice is $lpha_k:=rac{2}{L+\mu}.$

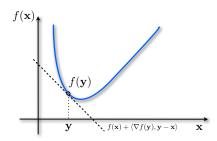
Case 3: If $f \in \mathcal{F}_2(\mathcal{Q})$, then, a bit more complicated (more later).

Towards a geometric interpretation I

Recall:

- Let $f \in \mathcal{F}^2_L(\mathbb{R}^p)$ with gradient $\nabla f(\mathbf{x})$ and Hessian $\nabla^2 f(\mathbf{x})$.
- ightharpoonup First-order Taylor approximation of f at y:

$$f(\mathbf{x}) \ge f(\mathbf{y}) + \langle \nabla f(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle$$



► Convex functions: 1st-order Taylor approximation is a global lower surrogate.

Towards a geometric interpretation II

Lemma

Let $f \in \mathcal{F}_L^{1,1}(\mathcal{Q})$. Then, we have:

$$f(\mathbf{y}) - f(\mathbf{x}) - \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \le \frac{L}{2} ||\mathbf{y} - \mathbf{x}||_2^2, \quad \forall \mathbf{x}, \mathbf{y} \in \mathcal{Q}.$$

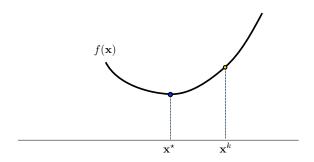
Proof.

By the Taylor's theorem:

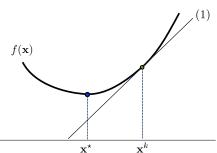
$$f(\mathbf{y}) = f(\mathbf{x}) + \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle + \int_0^1 \langle \nabla f(\mathbf{x} + \tau(\mathbf{y} - \mathbf{x})) - \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle d\tau.$$

Therefore,

$$f(\mathbf{y}) - f(\mathbf{x}) - \langle \nabla f(\mathbf{x}), \mathbf{y} - \mathbf{x} \rangle \le \int_0^1 \|\nabla f(\mathbf{x} + \tau(\mathbf{y} - \mathbf{x})) - \nabla f(\mathbf{x})\|^* \cdot \|\mathbf{y} - \mathbf{x}\| d\tau$$
$$\le L \|\mathbf{y} - \mathbf{x}\|_2^2 \int_0^1 \tau d\tau = \frac{L}{2} \|\mathbf{y} - \mathbf{x}\|_2^2$$







Structure in optimization:

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

Majorize:

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

$$\mathbf{Minimize:} \\ \mathbf{x}^{k+1} = \arg\min_{\mathbf{x}} Q_L(\mathbf{x}, \mathbf{x}^k)$$

$$= \arg\min_{\mathbf{x}} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L} \nabla f(\mathbf{x}^k) \right) \right\|^2$$

$$= \mathbf{x}^k - \frac{1}{L} \nabla f(\mathbf{x}^k)$$

$$(2)$$

$$\mathbf{f}(\mathbf{x})$$

$$= \mathbf{x}^k - \frac{1}{L} \nabla f(\mathbf{x}^k)$$

Structure in optimization:

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

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

 \mathbf{x}^{\star}

 $\mathbf{x}^{k+1}\mathbf{x}^k$

Majorize:

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

$$\mathbf{Minimize:}$$

$$\mathbf{x}^{k+1} = \arg\min_{\mathbf{x}} Q_{L'}(\mathbf{x}, \mathbf{x}^k)$$

$$= \arg\min_{\mathbf{x}} \left\| \mathbf{x} - \left(\mathbf{x}^k - \frac{1}{L'} \nabla f(\mathbf{x}^k) \right) \right\|^2$$

$$= \mathbf{x}^k - \frac{1}{L'} \nabla f(\mathbf{x}^k)$$
slower

Structure in optimization:

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

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





Majorize:

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

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

$$(1)$$

Structure in optimization:

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

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

(3)
$$f(\mathbf{x}) \ge f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{\mu}{2} ||\mathbf{x} - \mathbf{x}^k||_2^2$$

 \mathbf{x}^{\star}

 \mathbf{x}^k

Convergence rate of gradient descent

Theorem

$$\begin{split} & f \in \mathcal{F}_{L}^{2,1}, \quad \alpha = \frac{1}{L}: & f(\mathbf{x}^{k}) - f(\mathbf{x}^{\star}) \leq \frac{2L}{k+4} \|\mathbf{x}^{0} - \mathbf{x}^{\star}\|_{2}^{2} \\ & f \in \mathcal{F}_{L,\mu}^{2,1}, \quad \alpha = \frac{2}{L+\mu}: & \|\mathbf{x}^{k} - \mathbf{x}^{\star}\|_{2} \leq \left(\frac{L-\mu}{L+\mu}\right)^{k} \|\mathbf{x}^{0} - \mathbf{x}^{\star}\|_{2} \\ & f \in \mathcal{F}_{L,\mu}^{2,1}, \quad \alpha = \frac{1}{L}: & \|\mathbf{x}^{k} - \mathbf{x}^{\star}\|_{2} \leq \left(\frac{L-\mu}{L+\mu}\right)^{\frac{k}{2}} \|\mathbf{x}^{0} - \mathbf{x}^{\star}\|_{2} \end{split}$$

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

Convergence rate of gradient descent

Theorem

$$\begin{split} &f \in \mathcal{F}_L^{2,1}, \quad \alpha = \frac{1}{L}: & f(\mathbf{x}^k) - f(\mathbf{x}^\star) \leq \frac{2L}{k+4} \|\mathbf{x}^0 - \mathbf{x}^\star\|_2^2 \\ &f \in \mathcal{F}_{L,\mu}^{2,1}, \quad \alpha = \frac{2}{L+\mu}: & \|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^k \|\mathbf{x}^0 - \mathbf{x}^\star\|_2 \\ &f \in \mathcal{F}_{L,\mu}^{2,1}, \quad \alpha = \frac{1}{L}: & \|\mathbf{x}^k - \mathbf{x}^\star\|_2 \leq \left(\frac{L-\mu}{L+\mu}\right)^{\frac{k}{2}} \|\mathbf{x}^0 - \mathbf{x}^\star\|_2 \end{split}$$

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

Remarks

- ▶ Assumption: Lipschitz gradient. Result: convergence rate in objective values.
- Assumption: Strong convexity. Result: convergence rate in sequence of the iterates and in objective values.
- Note that the suboptimal step-size choice $\alpha=\frac{1}{L}$ adapts to the strongly convex case (i.e., it features a linear rate vs. the standard sublinear rate).

Example: Ridge regression

Optimization formulation

- Let $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$ given by $\mathbf{b} = \mathbf{A} \mathbf{x}^{\natural} + \mathbf{w}$, where $\mathbf{w} \in \mathbb{R}^n$ is some noise.
- ightharpoonup A classical estimator of \mathbf{x}^{\natural} , known as ridge regression, is

$$\min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x}) := \frac{1}{2} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2^2 + \frac{\rho}{2} \|\mathbf{x}\|_2^2.$$

where $\rho \geq 0$ is a regularization parameter

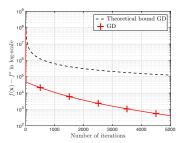
Remarks

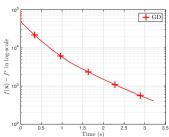
- $f \in \mathcal{F}_{L,\mu}^{2,1}$ with:
 - $L = \lambda_1(\mathbf{A}^T\mathbf{A}) + \rho;$
 - $\mu = \lambda_p(\mathbf{A}^T\mathbf{A}) + \rho;$
 - where $\lambda_1 \geq \ldots \geq \lambda_p$ are the eigenvalues of $\mathbf{A}^T \mathbf{A}$.
- ▶ The ratio $\kappa = \frac{L}{\mu}$ decreases as ρ increases, leading to faster linear convergence.
- ▶ Note that if n < p and $\rho = 0$, we have $\mu = 0$, hence $f \in \mathcal{F}_L^{2,1}$ and we can expect only $\mathcal{O}(1/k)$ convergence from the gradient descent method.

Example: Ridge regression

Case 1:

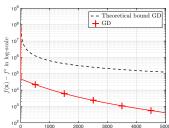
$$n = 500, \overline{p = 2000}, \rho = 0$$





Example: Ridge regression

Case_1: $n = 500, p = 2000, \rho = 0$



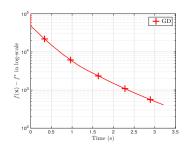
3000

Number of iterations

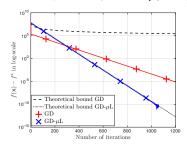
4000

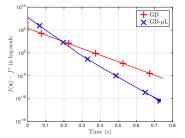
5000

1000



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





*From gradient descent to mirror descent

Gradient descent as a majorization-minimization scheme

▶ Majorize f at \mathbf{x}^k by using L-Lipschitz gradient continuity

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

Minimize $Q(\mathbf{x}, \mathbf{x}^k)$ to obtain the next iterate \mathbf{x}^{k+1}

$$\mathbf{x}^{k+1} = \operatorname*{arg\,min}_{\mathbf{x}} Q(\mathbf{x}, \mathbf{x}^k) \Rightarrow \nabla f(\mathbf{x}^k) + L(\mathbf{x}^{k+1} - \mathbf{x}^k) = 0$$
$$\mathbf{x}^{k+1} = \mathbf{x}^k - \frac{1}{I} \nabla f(\mathbf{x}^k)$$

Other majorizers

We can re-write the majorization step as

$$f(\mathbf{x}) \le f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \alpha d(\mathbf{x}, \mathbf{x}^k)$$

where $d(\mathbf{x}, \mathbf{x}^k) = \frac{1}{2} ||\mathbf{x} - \mathbf{x}^k||_2^2$ is the Euclidean distance and $\alpha = L$.

 \blacktriangleright Can we use a different function $d(\mathbf{x}, \mathbf{x}^k)$ that is better suited to minimizing f?

*Bregman divergences

Definition (Bregman divergence)

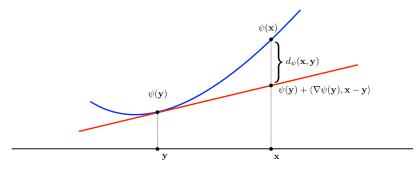
Let $\psi: \mathcal{S} \to \mathbb{R}$ be a continuously-differentiable and strictly convex function defined on a closed convex set \mathcal{S} . The **Bregman divergence** (d_{ψ}) associated with ψ for points \mathbf{x} and \mathbf{y} is:

$$d_{\psi}(\mathbf{x}, \mathbf{y}) = \psi(\mathbf{x}) - \psi(\mathbf{y}) - \langle \nabla \psi(\mathbf{y}), \mathbf{x} - \mathbf{y} \rangle$$

- $lackbox{}\psi(\cdot)$ is referred to as the Bregman or proximity function.
- ► The Bregman divergence satisfies the following properties:
 - (a) $d_{\psi}(\mathbf{x}, \mathbf{y}) \geq 0$ for all \mathbf{x} and \mathbf{y} with equality if and only if $\mathbf{x} = \mathbf{y}$
 - (b) Define $q(\mathbf{x}) := d_{\psi}(\mathbf{x}, \mathbf{y})$ for a fixed \mathbf{y} , then $\nabla q(\mathbf{x}) = \nabla \psi(\mathbf{x}) \nabla \psi(\mathbf{y})$
 - (c) For all $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{S}$, $d_{\psi}(\mathbf{x}, \mathbf{y}) = d_{\psi}(\mathbf{x}, \mathbf{z}) + d_{\psi}(\mathbf{z}, \mathbf{y}) + \langle (\mathbf{x} \mathbf{z}), \nabla \psi(\mathbf{y}) \nabla \psi(\mathbf{z}) \rangle$
 - (d) For all $\mathbf{x}, \mathbf{y} \in \mathcal{S}$, $d_{\psi}(\mathbf{x}, \mathbf{y}) + d_{\psi}(\mathbf{y}, \mathbf{x}) = \langle (\mathbf{x} \mathbf{y}), \nabla \psi(\mathbf{x}) \nabla \psi(\mathbf{y}) \rangle$
- ▶ The Bregman divergence becomes a Bregman distance when it is symmetric (i.e. $d_{\psi}(\mathbf{x}, \mathbf{y}) = d_{\psi}(\mathbf{y}, \mathbf{x})$) and satisfies the triangle inequality.
- ▶ "All Bregman distances are Bregman divergences but the reverse is not true!"

*Bregman divergences

The Bregman divergence is the vertical distance at x between ψ and the tangent of ψ at y, see figure below



▶ The Bregman divergence measures the strictness of convexity of $\psi(\cdot)$.

*Bregman divergences

Table: Bregman functions $\psi(\mathbf{x})$ & corresponding Bregman divergences/distances $d_{\psi}(\mathbf{x},\mathbf{y})^a$.

Name (or Loss)	Domain ^b	$\psi(\mathbf{x})$	$d_{\psi}(\mathbf{x}, \mathbf{y})$
Squared loss	R	x ²	$(x-y)^2$
Itakura-Saito divergence	R++	$-\log x$	$\frac{x}{y} - \log\left(\frac{x}{y}\right) - 1$
Squared Euclidean distance	\mathbb{R}^p	$\ \mathbf{x}\ _{2}^{2}$	$\ \mathbf{x} - \mathbf{y}\ _2^2$
Squared Mahalanobis distance	\mathbb{R}^p	$\langle \mathbf{x}, \mathbf{A} \mathbf{x} \rangle$	$\langle (\mathbf{x} - \mathbf{y}), \mathbf{A}(\mathbf{x} - \mathbf{y}) \rangle^{c}$
Entropy distance	p -simplex d	$\sum_{i} x_i \log x_i$	$\sum_{i} x_{i} \log \left(\frac{x_{i}}{y_{i}} \right)$
Generalized I-divergence	\mathbb{R}^p_+	$\sum_{i} x_i \log x_i$	$\sum_{i} \left(\log \left(\frac{x_i}{y_i} \right) - \left(x_i - y_i \right) \right)$
von Neumann divergence	$\mathbb{S}_{+}^{p \times p}$	$X \log X - X$	$\operatorname{tr} \left(\mathbf{X} \left(\log \mathbf{X} - \log \mathbf{Y} \right) - \mathbf{X} + \mathbf{Y} \right)^e$
logdet divergence	$\mathbb{S}_{+}^{p \times p}$	− log det X	$\operatorname{tr}\left(\mathbf{XY}^{-1}\right) - \log \det\left(\mathbf{XY}^{-1}\right) - p$

 $^{^{}a}~x,y\in\mathbb{R}\text{, }\mathbf{x},\mathbf{y}\in\mathbb{R}^{p}~\text{and}~\mathbf{X},\mathbf{Y}\in\mathbb{R}^{p\times p}.$

^d p-simplex:=
$$\{\mathbf{x} \in \mathbb{R}^p : \sum_{i=1}^p x_i = 1, x_i \ge 0, i = 1, \dots, p\}$$

 $[^]b$ \mathbb{R}_+ and \mathbb{R}_{++} denote non-negative and positive real numbers respectively.

 $^{^{}c}$ $\mathbf{A} \in \mathbb{S}_{+}^{p imes p}$, the set of symmetric positive semidefinite matrix.

 $^{^{}e}$ tr(${\bf A}$) is the trace of ${\bf A}$.

*Mirror descent [1]

What happens if we use a Bregman distance d_{ψ} in gradient descent?

Let $\psi: \mathbb{R}^p \to \mathbb{R}$ be a μ -strongly convex and continuously differentiable function and let the associated Bregman distance be $d_{\psi}(\mathbf{x},\mathbf{y}) = \psi(\mathbf{x}) - \psi(\mathbf{y}) - \langle \mathbf{x} - \mathbf{y}, \nabla \psi(\mathbf{y}) \rangle$. Assume that the inverse mapping ψ^{\star} of ψ is easily computable (i.e., its convex conjugate).

▶ Majorize: Find α_k such that

$$f(\mathbf{x}) \le f(\mathbf{x}^k) + \langle \nabla f(\mathbf{x}^k), \mathbf{x} - \mathbf{x}^k \rangle + \frac{1}{\alpha_k} d_{\psi}(\mathbf{x}, \mathbf{x}^k) := Q_{\psi}^k(\mathbf{x}, \mathbf{x}^k)$$

Minimize

$$\mathbf{x}^{k+1} = \underset{\mathbf{x}}{\arg\min} Q_{\psi}^{k}(\mathbf{x}, \mathbf{x}^{k}) \Rightarrow \nabla f(\mathbf{x}^{k}) + \frac{1}{\alpha_{k}} \left(\nabla \psi(\mathbf{x}^{k+1}) - \nabla \psi(\mathbf{x}^{k}) \right) = 0$$

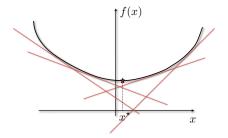
$$\nabla \psi(\mathbf{x}^{k+1}) = \nabla \psi(\mathbf{x}^{k}) - \alpha_{k} \nabla f(\mathbf{x}^{k})$$

$$\mathbf{x}^{k+1} = \nabla \psi^{*}(\nabla \psi(\mathbf{x}^{k}) - \alpha_{k} \nabla f(\mathbf{x}^{k})) \qquad (\nabla \psi(\cdot))^{-1} = \nabla \psi^{*}(\cdot)[4].$$

- Mirror descent is a generalization of gradient descent for functions that are Lipschitz-gradient in norms other than the Euclidean.
- \blacktriangleright MD allows to deal with some **constraints** via a proper choice of ψ .

*What to keep in mind about mirror descent?

ullet Approximates the optimum by lower bounding the function via hyperplanes at ${f x}_t$



• The smaller the gradients, the better the approximation!

*Mirror descent example

How can we minimize a convex function over the unit simplex?

$$\min_{\mathbf{x} \in \Delta} f(\mathbf{x}),$$

where

- lacksquare $\Delta:=\{\mathbf{x}\in\mathbb{R}^p : \sum_{j=1}^p x_j=1, \mathbf{x}\geq 0\}$ is the unit simplex;
- f is convex L_f -Lipschitz continuous with respect to some norm $\|\cdot\|$.

Entropy function

► Define the entropy function

$$\psi_e(\mathbf{x}) = \sum_{j=1}^p x_j \ln x_j$$
 if $\mathbf{x} \in \Delta$, $+\infty$ otherwise.

- ψ_e is 1-strongly convex over $\mathrm{int}\Delta$ with respect to $\|\cdot\|_1$.
- $\blacktriangleright \ \psi_e^{\star}(\mathbf{z}) = \ln \sum_{i=1}^p e^{z_j} \text{ and } \|\nabla \psi_e(\mathbf{x})\| \to \infty \text{ as } \mathbf{x} \to \tilde{\mathbf{x}} \in \Delta.$
- ▶ Let $\mathbf{x}^0 = p^{-1}\mathbf{1}$, then $d_{\psi}(\mathbf{x}, \mathbf{x}^0) \leq \ln p$ for all $\mathbf{x} \in \Delta$.

*Entropic descent algorithm [1]

Entropic descent algorithm (EDA)

Let $\mathbf{x}^0 = p^{-1}\mathbf{1}$ and generate the following sequence

$$x_j^{k+1} = \frac{x_j^k e^{-t_k f_j'(\mathbf{x}^k)}}{\sum_{j=1}^p x_j^k e^{-t_k f_j'(\mathbf{x}^k)}}, \quad t_k = \frac{\sqrt{2\ln p}}{L_f} \frac{1}{\sqrt{k}},$$

where $f'(\mathbf{x}) = (f_1(\mathbf{x})', \dots, f_p(\mathbf{x})')^T \in \partial f(\mathbf{x})$, which is the subdifferential of f at \mathbf{x} .

- This is an example of non-smooth and constrained optimization;
- ► The updates are multiplicative.

*Convergence of mirror descent

Problem

$$\min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}) \tag{1}$$

where

- $\triangleright \mathcal{X}$ is a closed convex subset of \mathbb{R}^p ;
- f is convex L_f -Lipschitz continuous with respect to some norm $\|\cdot\|$.

Theorem ([1])

Let $\{x^k\}$ be the sequence generated by mirror descent with $x^0\in \mathrm{int}\mathcal{X}$. If the step-sizes are chosen as

$$\alpha_k = \frac{\sqrt{2\mu d_{\psi}(\mathbf{x}^{\star}, \mathbf{x}^0)}}{L_f} \frac{1}{\sqrt{k}}$$

the following convergence rate holds

$$\min_{0 \le s \le k} f(\mathbf{x}^k) - f^* \le L_f \sqrt{\frac{2d_{\psi}(\mathbf{x}^*, \mathbf{x}^0)}{\mu}} \frac{1}{\sqrt{k}}$$

► This convergence rate is **optimal** for solving (1) with a first-order method.

Smooth unconstrained non-convex minimization

Problem (Mathematical formulation)

Let us consider the following problem formulation:

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

- f is a smooth and possibly non-convex function.
- Recall that finding the global minimizer, i.e., $f^* := \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x})$, is NP-hard

Example: Recall M-estimation

Problem: Binary classification

Let $(a_1,b_1),...,(a_n,b_n)$ be i.i.d. samples where a_i represent a feature vector and b_i its corresponding label (either 0 or 1). **Goal:** Learn a model that gives probability of assigning a particular label, given the feature vector.

Formulation (*M-estimator*)

Find the minimizing parameter for some "loss function", averaged over multiple samples.

$$\min_{x \in \mathcal{X}} \frac{1}{n} \sum_{i=1}^{n} l_i(a_i, b_i; \mathbf{x})$$

- ▶ What if we want to select a non-convex loss function?
- ▶ Why would we prefer a non-convex problem when convexity has nice properties?

Example: Recall M-estimation

Why non-convex?

- ▶ Inherent properties of optimization problem, e.g., phase retrieval
- ▶ Robustness or better estimation, e.g., binary classification with non-convex losses

Optimization Formulation: Phase Retrieval

$$\min_{x} |||Ax|^2 - b||_2^2$$

Optimization Formulation: Binary Classification

$$\min_{x} \left\{ \frac{1}{n} \sum_{i=1}^{n} (b_i - g(a_i, x))^2 \right\}$$

where $q(\cdot, \cdot)$ is non-linear, and hence, the loss function is non-convex.

Notion of convergence: Stationarity

ullet Let $f(\mathbf{x}): \mathbb{R}^d o \mathbb{R}$ be a twice-differentiable and $\mathbf{x}^\star = \min_{x \in \mathbb{R}^d} f(\mathbf{x})$

Definition (Recall - First order stationary point)

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

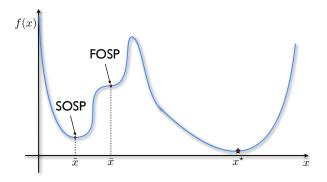
$$\nabla f(\bar{\mathbf{x}}) = \mathbf{0}.$$

Definition (Recall - Second order stationary point)

A point $ilde{\mathbf{x}}$ is a second order stationary point of a twice differentiable function $f(\mathbf{x})$ if

$$\nabla f(\tilde{\mathbf{x}}) = \mathbf{0} \quad \text{and} \quad \nabla^2 f(\tilde{\mathbf{x}}) \succeq \mathbf{0}.$$

Geometric interpretation of stationarity



• Note that neither $\bar{\mathbf{x}}$, nor $\tilde{\mathbf{x}}$ is **not necessarily** equal to \mathbf{x}^{\star} !!

Assumptions and the gradient method

Assumption: Smoothness

Let $f \in \mathcal{F}_L^{2,1}$ and has L-Lipschitz gradient with respect to ℓ_2 norm, such that,

$$||\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})||_2 \le L||\mathbf{x} - \mathbf{y}||$$

Gradient descent

Let $\alpha \leq \frac{1}{L}$ be the constant step size and $\mathbf{x}^0 \in \mathsf{dom}(f)$ be the initial point. Then, gradient method produces iterates using the following iterative update,

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

Convergence rate and iteration complexity

Theorem

Let $f \in \mathcal{F}_L^{2,1}$, and $\alpha \leq \frac{1}{L}$. Then, gradient method converges to the FOSP with the following properties:

Convergence rate to an ϵ -FOSP:

$$\|\nabla f(\mathbf{x}^t)\| = O\left(\frac{1}{\sqrt{t}}\right)$$

Iteration complexity to reach an ϵ -FOSP:

$$O\left(\frac{1}{\epsilon^2}\right)$$

Example: Phase retrieval for fourier pytchography

Definition (Phase retrieval)

Given a set of measurements of the amplitude of a signal, phase retrieval is the task of finding the phase for the original signal that satisfies certain constraints/properties.

Definition (Fourier ptychography)

Fourier ptychography is the task of reconstructing high-resolution images from low resolution samples, based on optical microscopy. It is a special case of phase retrieval problem.

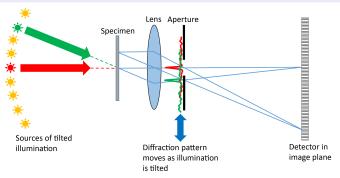
Example: Phase retrieval for fourier pytchography

Definition (Phase retrieval)

Given a set of measurements of the amplitude of a signal, phase retrieval is the task of finding the phase for the original signal that satisfies certain constraints/properties.

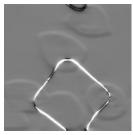
Definition (Fourier ptychography)

Fourier ptychography is the task of reconstructing high-resolution images from low resolution samples, based on optical microscopy. It is a special case of phase retrieval problem.

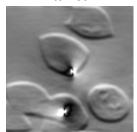


Example: Malaria infection detection

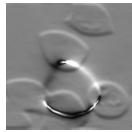
iter: 1



iter: 80



iter: 40



iter: 120



Example: Image classification using neural networks

Recall: Neural network formulation

- $ightharpoonup ({f a}_i,b_i)$: sample points, $\sigma(\cdot)$: non-linear activation function
- lacktriangle the function class $\mathcal F$ is given by $\mathcal F:=\left\{g(\cdot,\cdot),\mathbf x\in\mathbb R^d\right\}$, where

$$\mathbf{x} = (W_1, c_1, W_2, c_2, \dots, W_k, c_k), \quad W_i \in \mathbb{R}^{d_i \times d_{i-1}}, \quad c_i \in \mathbb{R}^{d_i},$$
$$g(\mathbf{a}, \mathbf{x}) = \sigma(W_k \sigma(\cdots \sigma(W_2 \sigma(W_1 \mathbf{a} + c_1) + c_2) \cdots) + c_k)$$

▶ the loss function is given by $L(g(\mathbf{a}, \mathbf{x}), b) := (b - g(\mathbf{a}, \mathbf{x}))^2$.

Example: Image classification



Imagenet: 1000 object classes. 1.2M/100K train/test images Below human level error rates!

References |

[1] Amir Beck and Marc Teboulle.

Mirror descent and nonlinear projected subgradient methods for convex optimization.

Operations Research Letters, 31(3):167-175, 2003.

[2] Lucien Le Cam.

Asymptotic methods in Statistical Decision Theory. Springer-Verl., New York, NY, 1986.

[3] Yu. Nesterov.

Introductory Lectures on Convex Optimization: A Basic Course. Kluwer. Boston. MA. 2004.

[4] R.T. Rockafellar.

Convex analysis.

Princeton University Press (Princeton, NJ), 1970.

[5] A. W. van der Vaart.

Asymptotic Statistics.

Cambridge Univ. Press, Cambridge, UK, 1998.