

Introduction to nonconvex optimization



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Unconstrained optimization

Consider an unconstrained optimization problem

$$\text{minimize}_{\mathbf{x}} \quad f(\mathbf{x})$$

- For simplicity, we assume $f(\mathbf{x})$ is twice differentiable
- We assume the minimizer \mathbf{x}_{opt} exists, i.e.,

$$\mathbf{x}_{\text{opt}} := \arg \min_{\mathbf{x}} f(\mathbf{x})$$

Critical/stationary points

Definition 7.1

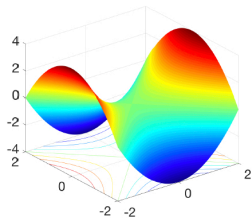
A first-order critical point of f satisfies

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

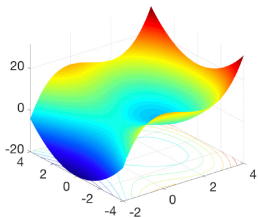
- If f is convex, any 1st-order critical point is a global minimizer
- Finding 1st-order stationary point is sufficient for convex optimization
- Example: gradient descent (GD)

How about nonconvex optimization?

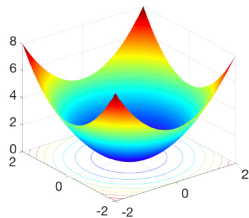
First-order critical points could be global min, local min, local max, saddle points...



(a) strict saddle



(b) local minimum



(c) global minimum

figure credit: Li et al. '16

Simple algorithms like GD could stuck at undesired stationary points

Types of critical points

Definition 7.2

A second-order critical point \mathbf{x} satisfies

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

For any first-order critical point \mathbf{x} :

- $\nabla^2 f(\mathbf{x}) \prec \mathbf{0}$ \rightarrow local maximum
- $\nabla^2 f(\mathbf{x}) \succ \mathbf{0}$ \rightarrow local minimum
- $\lambda_{\min}(\nabla^2 f(\mathbf{x})) < 0$ \rightarrow *strict saddle point*

When are nonconvex problems solvable?

(Local) strong convexity and smoothness

Definition 7.3

A twice differentiable function $f : \mathbb{R}^n \mapsto \mathbb{R}$ is said to be α -strongly convex in a set \mathcal{B} if for all $\mathbf{x} \in \mathcal{B}$

$$\nabla^2 f(\mathbf{x}) \succeq \alpha \mathbf{I}_n.$$

Definition 7.4

A twice differentiable function $f : \mathbb{R}^n \mapsto \mathbb{R}$ is said to be β -smooth in a set \mathcal{B} if for all $\mathbf{x} \in \mathcal{B}$

$$\|\nabla^2 f(\mathbf{x})\| \leq \beta.$$

Gradient descent theory revisited

Gradient descent method with step size $\eta > 0$

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

Lemma 7.5

Suppose f is α -strongly convex and β -smooth in the local ball $\mathcal{B}_\delta(\mathbf{x}_{\text{opt}}) := \{\mathbf{x} \mid \|\mathbf{x} - \mathbf{x}_{\text{opt}}\|_2 \leq \delta\}$. Running gradient descent from $\mathbf{x}^0 \in \mathcal{B}_\delta(\mathbf{x}_{\text{opt}})$ with $\eta = 1/\beta$ achieves linear convergence

$$\|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2 \leq \left(1 - \frac{\alpha}{\beta}\right)^t \|\mathbf{x}^0 - \mathbf{x}_{\text{opt}}\|_2, \quad t = 0, 1, 2, \dots$$

Implications

- Condition number β/α determines rate of convergence
- Attains ε -accuracy (i.e., $\|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2 \leq \varepsilon\|\mathbf{x}_{\text{opt}}\|_2$) within

$$O\left(\frac{\beta}{\alpha} \log \frac{1}{\varepsilon}\right)$$

iterations

- Needs initialization $\mathbf{x}^0 \in \mathcal{B}_\delta(\mathbf{x}_{\text{opt}})$: basin of attraction

Proof of Lemma 7.5

Since $\nabla f(\mathbf{x}_{\text{opt}}) = \mathbf{0}$, we can rewrite GD as

$$\begin{aligned}\mathbf{x}^{t+1} - \mathbf{x}_{\text{opt}} &= \mathbf{x}^t - \eta \nabla f(\mathbf{x}^t) - [\mathbf{x}_{\text{opt}} - \eta \nabla f(\mathbf{x}_{\text{opt}})] \\ &= \left[\mathbf{I}_n - \eta \int_0^1 \nabla^2 f(\mathbf{x}(\tau)) d\tau \right] (\mathbf{x}^t - \mathbf{x}_{\text{opt}}),\end{aligned}$$

where $\mathbf{x}(\tau) := \mathbf{x}_{\text{opt}} + \tau(\mathbf{x}^t - \mathbf{x}_{\text{opt}})$. By local strong convexity and smoothness, one has

$$\alpha \mathbf{I}_n \preceq \nabla^2 f(\mathbf{x}(\tau)) \preceq \beta \mathbf{I}_n, \quad \text{for all } 0 \leq \tau \leq 1$$

Therefore $\eta = 1/\beta$ yields

$$\mathbf{0} \preceq \mathbf{I}_n - \eta \int_0^1 \nabla^2 f(\mathbf{x}(\tau)) d\tau \preceq \left(1 - \frac{\alpha}{\beta}\right) \mathbf{I}_n,$$

which further implies

$$\|\mathbf{x}^{t+1} - \mathbf{x}_{\text{opt}}\|_2 \leq \left(1 - \frac{\alpha}{\beta}\right) \|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2$$

Regularity condition

More generally, for update rule

$$\mathbf{x}^{t+1} = \mathbf{x}^t - \eta \mathbf{g}(\mathbf{x}^t),$$

where $g(\cdot) : \mathbb{R}^n \mapsto \mathbb{R}^n$

Definition 7.6

$g(\cdot)$ is said to obey RC(μ, λ, δ) for some $\mu, \lambda, \delta > 0$ if

$$2\langle \mathbf{g}(\mathbf{x}), \mathbf{x} - \mathbf{x}_{\text{opt}} \rangle \geq \mu \|\mathbf{g}(\mathbf{x})\|_2^2 + \lambda \|\mathbf{x} - \mathbf{x}_{\text{opt}}\|_2^2 \quad \forall \mathbf{x} \in \mathcal{B}_\delta(\mathbf{x}_{\text{opt}})$$

- Negative search direction \mathbf{g} is positively correlated with error $\mathbf{x} - \mathbf{x}_{\text{opt}} \implies$ one-step improvement
- $\mu\lambda \leq 1$ by Cauchy-Schwarz

RC = one-point strong convexity + smoothness

- One-point α -strong convexity:

$$f(\mathbf{x}_{\text{opt}}) - f(\mathbf{x}) \geq \langle \nabla f(\mathbf{x}), \mathbf{x}_{\text{opt}} - \mathbf{x} \rangle + \frac{\alpha}{2} \|\mathbf{x} - \mathbf{x}_{\text{opt}}\|_2^2 \quad (7.1)$$

- β -smoothness:

$$\begin{aligned} f(\mathbf{x}_{\text{opt}}) - f(\mathbf{x}) &\leq f\left(\mathbf{x} - \frac{1}{\beta} \nabla f(\mathbf{x})\right) - f(\mathbf{x}) \\ &\leq \left\langle \nabla f(\mathbf{x}), -\frac{1}{\beta} \nabla f(\mathbf{x}) \right\rangle + \frac{\beta}{2} \left\| \frac{1}{\beta} \nabla f(\mathbf{x}) \right\|_2^2 \\ &= -\frac{1}{2\beta} \|\nabla f(\mathbf{x})\|_2^2 \end{aligned} \quad (7.2)$$

RC = one-point strong convexity + smoothness

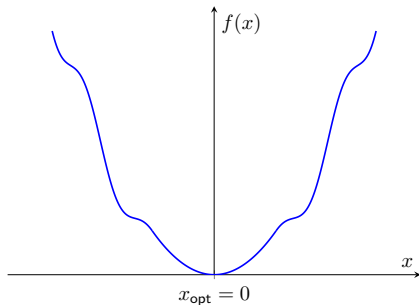
Combining relations (7.1) and (7.2) yields

$$\langle \nabla f(\mathbf{x}), \mathbf{x} - \mathbf{x}_{\text{opt}} \rangle \geq \frac{\alpha}{2} \|\mathbf{x} - \mathbf{x}_{\text{opt}}\|_2^2 + \frac{1}{2\beta} \|\nabla f(\mathbf{x})\|_2^2$$

— *RC holds with $\mu = 1/\beta$ and $\lambda = \alpha$*

Example of nonconvex functions

When $\mathbf{g}(x) = \nabla f(x)$, f is not necessarily convex



$$f(x) = \begin{cases} x^2, & |x| \leq 6, \\ x^2 + 1.5|x|(\cos(|x| - 6) - 1), & |x| > 6 \end{cases}$$

Convergence under RC

Lemma 7.7

Suppose $g(\cdot)$ obeys $\text{RC}(\mu, \lambda, \delta)$. The update rule $(\mathbf{x}^{t+1} = \mathbf{x}^t - \eta \mathbf{g}(\mathbf{x}^t))$ with $\eta = \mu$ and $\mathbf{x}^0 \in \mathcal{B}_\delta(\mathbf{x}_{\text{opt}})$ obeys

$$\|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2^2 \leq (1 - \mu\lambda)^t \|\mathbf{x}^0 - \mathbf{x}_{\text{opt}}\|_2^2$$

- $\mathbf{g}(\cdot)$: more general search directions
 - example: in vanilla GD, $\mathbf{g}(\mathbf{x}) = \nabla f(\mathbf{x})$
- The product $\mu\lambda$ determines the rate of convergence
- Attains ε -accuracy within $O\left(\frac{1}{\mu\lambda} \log \frac{1}{\varepsilon}\right)$ iterations

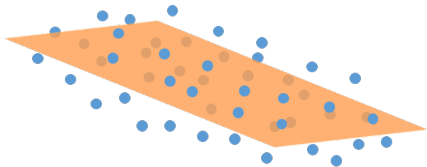
Proof of Lemma 7.7

By definition, one has

$$\begin{aligned}\|\mathbf{x}^{t+1} - \mathbf{x}_{\text{opt}}\|_2^2 &= \|\mathbf{x}^t - \eta \mathbf{g}(\mathbf{x}^t) - \mathbf{x}_{\text{opt}}\|_2^2 \\ &= \|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2^2 + \eta^2 \|\mathbf{g}(\mathbf{x}^t)\|_2^2 - 2\eta \langle \mathbf{g}(\mathbf{x}^t), \mathbf{x}^t - \mathbf{x}_{\text{opt}} \rangle \\ &\leq \|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2^2 + \eta^2 \|\mathbf{g}(\mathbf{x}^t)\|_2^2 - \eta \left(\lambda \|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2^2 + \mu \|\mathbf{g}(\mathbf{x}^t)\|_2^2 \right) \\ &= (1 - \eta\lambda) \|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2^2 + \eta(\eta - \mu) \|\mathbf{g}(\mathbf{x}^t)\|_2^2 \\ &\leq (1 - \mu\lambda) \|\mathbf{x}^t - \mathbf{x}_{\text{opt}}\|_2^2\end{aligned}$$

A toy example: rank-1 matrix factorization

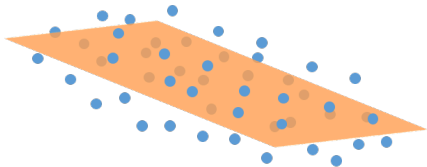
Principal component analysis



Given $M \succeq \mathbf{0} \in \mathbb{R}^{n \times n}$ (not necessarily low-rank), find its best rank- r approximation:

$$\widehat{M} = \underbrace{\operatorname{argmin}_{\mathbf{Z}} \|\mathbf{Z} - M\|_F^2}_{\text{nonconvex optimization!}} \quad \text{s.t.} \quad \operatorname{rank}(\mathbf{Z}) \leq r$$

Principal component analysis



This problem admits a closed-form solution

- let $M = \sum_{i=1}^n \lambda_i \mathbf{u}_i \mathbf{u}_i^\top$ be eigen-decomposition of M ($\lambda_1 \geq \dots \geq \lambda_r > \lambda_{r+1} \geq \dots \geq \lambda_n$), then

$$\widehat{M} = \sum_{i=1}^r \lambda_i \mathbf{u}_i \mathbf{u}_i^\top$$

— *nonconvex, but tractable*

Optimization viewpoint

If we factorize $\mathbf{Z} = \mathbf{X}\mathbf{X}^\top$ with $\mathbf{X} \in \mathbb{R}^{n \times r}$, then it leads to a nonconvex problem:

$$\text{minimize}_{\mathbf{X} \in \mathbb{R}^{n \times r}} f(\mathbf{X}) = \frac{1}{4} \|\mathbf{X}\mathbf{X}^\top - \mathbf{M}\|_{\text{F}}^2$$

To simplify exposition, set $r = 1$:

$$\text{minimize}_{\mathbf{x}} f(\mathbf{x}) = \frac{1}{4} \|\mathbf{x}\mathbf{x}^\top - \mathbf{M}\|_{\text{F}}^2$$

Interesting questions

$$\text{minimize}_{\mathbf{x} \in \mathbb{R}^n} f(\mathbf{x}) = \frac{1}{4} \|\mathbf{x}\mathbf{x}^\top - \mathbf{M}\|_{\text{F}}^2$$

- What does the curvature behave like, at least locally around the global minimizer?
- Where / what are the critical points? (Global geometry)

Local linear convergence of GD

Theorem 7.8

Suppose that $\|\mathbf{x}_0 - \sqrt{\lambda_1}\mathbf{u}_1\|_2 \leq \frac{\lambda_1 - \lambda_2}{15\sqrt{\lambda_1}}$ and set $\eta = \frac{1}{4.5\lambda_1}$, GD obeys

$$\|\mathbf{x}^t - \sqrt{\lambda_1}\mathbf{u}_1\|_2 \leq \left(1 - \frac{\lambda_1 - \lambda_2}{18\lambda_1}\right)^t \|\mathbf{x}^0 - \sqrt{\lambda_1}\mathbf{u}_1\|_2, \quad t \geq 0,$$

- condition number/eigengap determines rate of convergence
- Requires initialization: use spectral method?

Proof of Theorem 7.8

It suffices to show that for all \mathbf{x} obeying $\underbrace{\|\mathbf{x} - \sqrt{\lambda_1}\mathbf{u}_1\|_2}_{\text{basin of attraction}} \leq \frac{\lambda_1 - \lambda_2}{15\sqrt{\lambda_1}}$,

$$0.25(\lambda_1 - \lambda_2)\mathbf{I}_n \preceq \nabla^2 f(\mathbf{x}) \preceq 4.5\lambda_1\mathbf{I}_n$$

Express gradient and Hessian as

$$\begin{aligned}\nabla f(\mathbf{x}) &= (\mathbf{x}\mathbf{x}^\top - \mathbf{M})\mathbf{x} \\ \nabla^2 f(\mathbf{x}) &= 2\mathbf{x}\mathbf{x}^\top + \|\mathbf{x}\|_2^2\mathbf{I}_n - \mathbf{M}\end{aligned}$$

Preliminary facts

Let $\Delta := \mathbf{x} - \sqrt{\lambda_1} \mathbf{u}_1$. It is seen that when $\|\Delta\|_2 \leq \frac{\lambda_1 - \lambda_2}{15\sqrt{\lambda_1}}$, one has

$$\lambda_1 - 0.25(\lambda_1 - \lambda_2) \leq \|\mathbf{x}\|_2^2 \leq 1.15\lambda_1;$$

$$\|\Delta\|_2 \leq \|\mathbf{x}\|_2;$$

$$\|\Delta\|_2 \|\mathbf{x}\|_2 \leq (\lambda_1 - \lambda_2)/12$$

Local smoothness

Triangle inequality gives

$$\begin{aligned}\|\nabla^2 f(\mathbf{x})\| &\leq \|2\mathbf{x}\mathbf{x}^\top\| + \|\mathbf{x}\|_2^2 + \|\mathbf{M}\| \\ &\leq 3\|\mathbf{x}\|_2^2 + \lambda_1 < 4.5\lambda_1,\end{aligned}$$

where the last relation follows from $\|\mathbf{x}\|_2^2 \leq 1.15\lambda_1$

Local strong convexity

Recall that $\Delta = x - \sqrt{\lambda_1}u_1$

$$\begin{aligned}xx^\top &= \lambda_1 u_1 u_1^\top + \Delta x^\top + x \Delta^\top - \Delta \Delta^\top \\ &\succeq \lambda_1 u_1 u_1^\top - 3\|\Delta\|_2\|x\|_2 I_n \quad (\|\Delta\|_2 \leq \|x\|_2) \\ &\succeq \lambda_1 u_1 u_1^\top - 0.25(\lambda_1 - \lambda_2)I_n,\end{aligned}$$

where last line relies on $\|\Delta\|_2\|x\|_2 \leq (\lambda_1 - \lambda_2)/12$. Consequently,

$$\begin{aligned}\nabla^2 f(x) &= 2xx^\top + \|x\|_2^2 I_n - \lambda_1 u_1 u_1^\top - \sum_{i=2}^n \lambda_i u_i u_i^\top \\ &\succeq 2\lambda_1 u_1 u_1^\top + (\|x\|_2^2 - 0.5)(\lambda_1 - \lambda_2)I_n - \lambda_1 u_1 u_1^\top - \sum_{i=2}^n \lambda_i u_i u_i^\top \\ &\succeq (\|x\|_2^2 - 0.5(\lambda_1 - \lambda_2) + \lambda_1)u_1 u_1^\top \\ &\quad + \sum_{i=2}^n (\|x\|_2^2 - 0.5(\lambda_1 - \lambda_2) - \lambda_i)u_i u_i^\top \\ &\succeq (\|x\|_2^2 - 0.5(\lambda_1 - \lambda_2) - \lambda_2)I_n \\ &\succeq 0.25(\lambda_1 - \lambda_2)I_n \quad (\lambda_1 - 0.25(\lambda_1 - \lambda_2) \leq \|x\|_2^2)\end{aligned}$$

Critical points of $f(\cdot)$

\mathbf{x} is a critical point, i.e., $\nabla f(\mathbf{x}) = (\mathbf{x}\mathbf{x}^\top - \mathbf{M})\mathbf{x} = \mathbf{0}$

\Leftrightarrow

$$\mathbf{M}\mathbf{x} = \|\mathbf{x}\|_2^2 \mathbf{x}$$

\Leftrightarrow

\mathbf{x} aligns with an eigenvector of \mathbf{M} or $\mathbf{x} = \mathbf{0}$

Since $\mathbf{M}\mathbf{u}_i = \lambda_i \mathbf{u}_i$, the set of critical points is given by

$$\{\mathbf{0}\} \cup \{\pm\sqrt{\lambda_i} \mathbf{u}_i, \quad i = 1, \dots, n\}$$

Categorization of critical points

The critical points can be further categorized based on the **Hessian**:

$$\nabla^2 f(\mathbf{x}) = 2\mathbf{x}\mathbf{x}^\top + \|\mathbf{x}\|_2^2 \mathbf{I}_n - \mathbf{M}$$

- For any non-zero critical point $\mathbf{x}_k = \pm\sqrt{\lambda_k}\mathbf{u}_k$:

$$\begin{aligned}\nabla^2 f(\mathbf{x}_k) &= 2\lambda_k \mathbf{u}_k \mathbf{u}_k^\top + \lambda_k \mathbf{I} - \mathbf{M} \\ &= 2\lambda_k \mathbf{u}_k \mathbf{u}_k^\top + \lambda_k \left(\sum_{i=1}^n \mathbf{u}_i \mathbf{u}_i^\top \right) - \sum_{i=1}^n \lambda_i \mathbf{u}_i \mathbf{u}_i^\top \\ &= \sum_{i:i \neq k} (\lambda_k - \lambda_i) \mathbf{u}_i \mathbf{u}_i^\top + 2\lambda_k \mathbf{u}_k \mathbf{u}_k^\top\end{aligned}$$

Categorization of critical points (cont.)

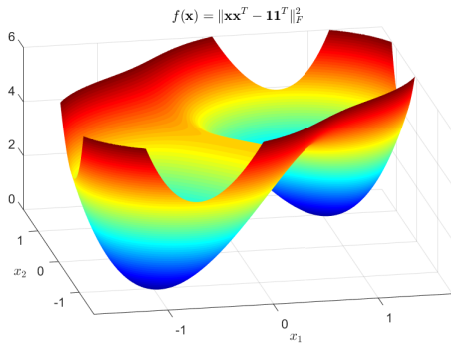
If $\lambda_1 > \lambda_2 \geq \dots \geq \lambda_n \geq 0$, then

- $\nabla^2 f(\mathbf{x}_1) \succ \mathbf{0} \quad \rightarrow \quad \text{local minima}$
- $1 < k \leq n: \lambda_{\min}(\nabla^2 f(\mathbf{x}_k)) < 0, \lambda_{\max}(\nabla^2 f(\mathbf{x}_k)) > 0$
 $\quad \quad \quad \rightarrow \quad \text{strict saddle}$
- $\mathbf{x} = \mathbf{0}: \nabla^2 f(\mathbf{0}) = -\mathbf{M} \preceq \mathbf{0} \quad \rightarrow \quad \text{local maxima, strict saddle}$

all local are global; all saddle are strict

A pictorial example

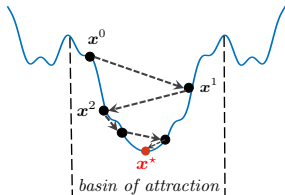
For example, for 2-dimensional case $f(\mathbf{x}) = \left\| \mathbf{x}\mathbf{x}^\top - \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \right\|_F^2$



global minima: $\mathbf{x} = \pm \begin{bmatrix} 1 \\ 1 \end{bmatrix}$; strict saddles: $\mathbf{x} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$, and $\pm \begin{bmatrix} 1 \\ -1 \end{bmatrix}$
— No “spurious” local minima!

Two vignettes

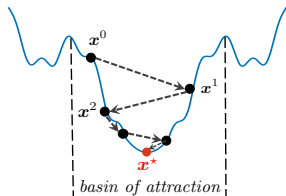
Two-stage approach:



smart initialization
+
local refinement

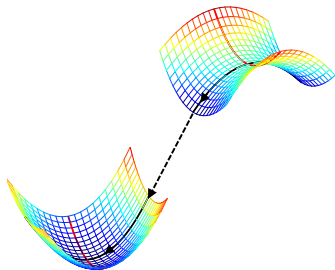
Two vignettes

Two-stage approach:



smart initialization
+
local refinement

Global landscape:



benign landscape
+
saddle-point escaping

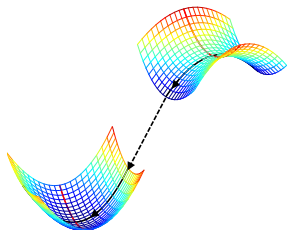
Global landscape

Benign landscape:

- all local minima = global minima
- other critical points = strict saddle points

Saddle-point escaping algorithms:

- trust-region methods
- perturbed gradient descent
- perturbed SGD
- ...



Next steps

- Generic local analysis of (regularized) gradient descent
- Refined local analysis for gradient descent
- Global landscape analysis
- Gradient descent with random initialization
- (Maybe) Gradient descent with arbitrary initialization