Session 11: Optimality conditions

Optimization and Computational Linear Algebra for Data Science

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1. Critical points (Unconstrained optimization)

Definitions

Definition

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a differentiable function. We say that $x \in \mathbb{R}^n$ is

- a critical point of f if $\nabla f(x) = 0$,
- a *global* minimizer of f if for all $x' \in \mathbb{R}^n$, $f(x) \leq f(x')$,
- a *local* minimizer of f if there exists $\delta > 0$ such that we have $f(x) \leq f(x')$ for all x' verifying $\|x - x'\| \leq \delta$.

1.1 Local extrema

Proposition

$$x \text{ is a local minimizer of } f \implies \nabla f(x) = 0.$$

Proposition

Assume that f is convex. Then

$$\nabla f(x) = 0 \iff x \text{ is a global minimizer of } f.$$

Looking at the Hessian

Proposition

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a twice differentiable function. Let $x \in \mathbb{R}^n$ be a critical point of f, i.e. $\nabla f(x) = 0$.
Then, if $H_f(x)$ is positive definite (that is, if all the eigenvalues of $H_f(x)$ are strictly positive), then x is a local minimizer of f.

Looking at the Hessian

Proposition

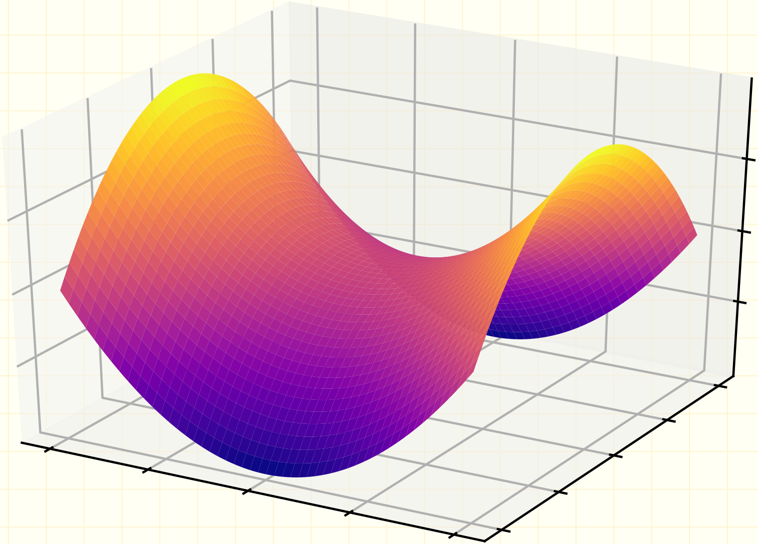
Let $f : \mathbb{R}^n \to \mathbb{R}$ be a twice differentiable function. Let $x \in \mathbb{R}^n$ be a critical point of f, i.e. $\nabla f(x) = 0$.
Then, if $H_f(x)$ is negative definite (that is, if all the eigenvalues of $H_f(x)$ are strictly negative), then x is a local maximizer of f.

1.2 Saddle points

Proposition

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a twice differentiable function. Let $x \in \mathbb{R}^n$ be a critical point of f, i.e. $\nabla f(x) = 0$.
Then, if $H_f(x)$ admits strictly positive eigenvalues and strictly negative eigenvalues, then x is neither a local maximum nor a local minimum. We call x a saddle point.

1.2 Saddle points



1.3 Examples

Study the critical points of $f(x, y) = x^2 + xy^2 - x + 1$.

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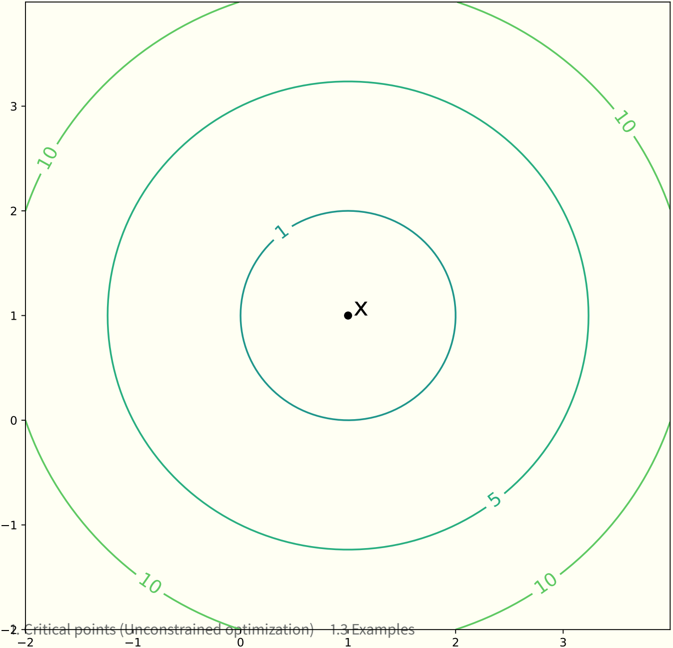
Critical points' critical points

- Global minimizer $\implies$ local minimizer $\implies$ critical point.

- Critical point + positive definite Hessian $\implies$ local minimizer.

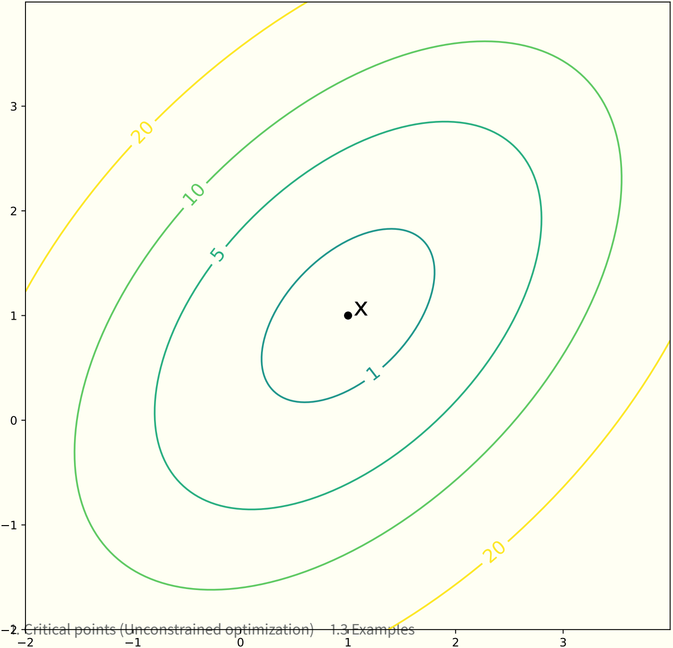
Example: Hessian at critical point



The eigenvalues of the Hessian at x are

1. $\begin{cases} \lambda_1 = 1 \\ \lambda_2 = -1 \end{cases}$
2. $\begin{cases} \lambda_1 = 1 \\ \lambda_2 = 1 \end{cases}$
3. $\begin{cases} \lambda_1 = 2 \\ \lambda_2 = 1 \end{cases}$
4. $\begin{cases} \lambda_1 = -1 \\ \lambda_2 = -1 \end{cases}$

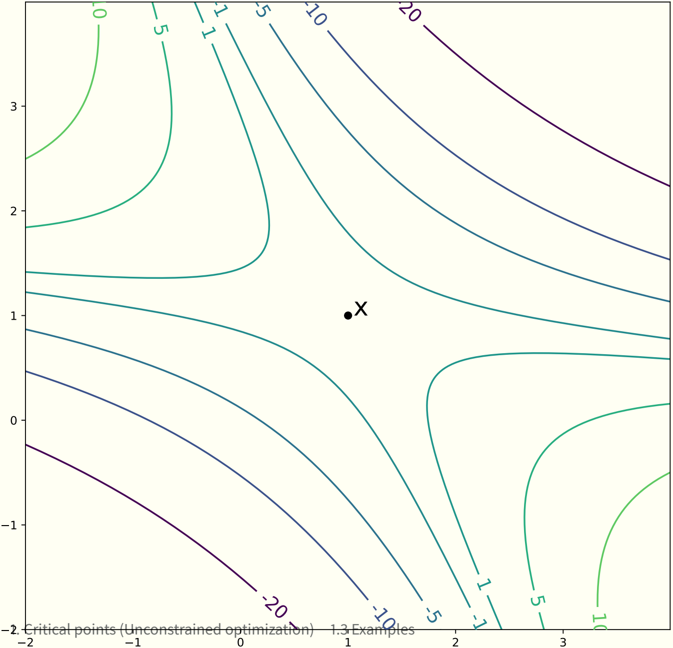
Example: Hessian at critical point



The eigenvalues of the Hessian at x are

1. $\begin{cases} \lambda_1 = 1 \\ \lambda_2 = -3 \end{cases}$
2. $\begin{cases} \lambda_1 = 2 \\ \lambda_2 = 2 \end{cases}$
3. $\begin{cases} \lambda_1 = 1 \\ \lambda_2 = 3 \end{cases}$
4. $\begin{cases} \lambda_1 = -1 \\ \lambda_2 = -1 \end{cases}$

Example: Hessian at critical point



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3. $\begin{cases} \lambda_1 = 1 \\ \lambda_2 = 3 \end{cases}$
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2. Constrained optimization

General formulation

Constrained optimization problems take the form:

$$
\begin{array}{lll}
\text{minimize} & f(x) & \text{with variable } x \in \mathbb{R}^n. \\
\\
\text{subject to} & g_i(x) \leq 0, & i = 1, \ldots, m \\
 & h_i(x) = 0, & i = 1, \ldots, p,
\end{array}
$$

Example:

2.1 Feasible points

Definition

A point $x \in \mathbb{R}^n$ is *feasible* if it satisfies all the constraints:
$g_1(x) \leq 0, \ldots, g_m(x) \leq 0$ and $h_1(x) = 0, \ldots, h_p(x) = 0$.

Example:

Question

If x is a solution to

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p, \end{array}$$

do we have $\nabla f(x) = 0$?

2.2 First order optimality condition

Consider the following problem:

$$\text{minimize} \quad f(x) \quad \text{subject to} \quad g_(x) \leq 0 \qquad (\star)$$

Case 1: “x inside”

- There exists $\delta > 0$ such that $B(x, \delta) \subset F$.

Case 2: "x on boundary"

- The constraint is active at x: $g(x) = 0$.

Cases summary

Case 1: "x inside" $\Rightarrow \nabla f(x) = 0$.

Case 2: active constraint, $g(x) = 0 \Rightarrow \nabla f(x) = -\lambda \nabla g(x)$ for $\lambda \geq 0$

.

First order optimality condition

Theorem

If x is a solution and if $\nabla h_1(x), \dots, \nabla h_p(x), \{\nabla g_i(x) \mid g_i(x) = 0\}$ are linearly independent, then there exists $\lambda_1, \dots, \lambda_m \geq 0$ and $\nu_1, \dots, \nu_p \in \mathbb{R}$ such that:

$$\nabla f(x) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x) + \sum_{i=1}^{p} \nu_i \nabla h_i(x) = 0.$$

Moreover, for all $i \in \{1, \dots, m\}$, if $g_i(x) < 0$ then $\lambda_i = 0$.

Example

Let $u \in \mathbb{R}^n$ be a non-zero vector.

$$\begin{array}{ll} \text{Minimize} & \langle x, u \rangle \\ \text{subject to} & \|x\|^2 = 1. \end{array}$$

Example

Let $u \in \mathbb{R}^n$ be a non-zero vector.

$$\begin{array}{ll} \text{Minimize} & \langle x, u \rangle \\ \text{subject to} & \|x\|^2 = 1. \end{array}$$

3. Convex constrained optimization

General formulation

We say that the constrained optimization problem

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_i(x) = 0, \quad i = 1, \ldots, p, \end{array}$$

is convex when $f, g_1, \ldots, g_m$ are convex and $h_1, \ldots, h_p$ are affine.

Karush-Kuhn-Tucker Theorem

Theorem (KKT)

Assume that the problem is convex and that there exists a feasible point x_0 such that $g_i(x_0) < 0$ for all i.
Then x is a solution if and only if x is feasible and there exists $\lambda_1, \dots, \lambda_m \geq 0, \nu_1, \dots, \nu_p \in \mathbb{R}$ such that:

$$\begin{cases} \nabla f(x) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x) + \sum_{i=1}^{p} \nu_i \nabla h_i(x) = 0. \\ \lambda_i g_i(x) = 0, \ \text{ for all } \ i \in \{1, \dots, p\}. \end{cases}$$

Example: Ridge regression

$$
\begin{array}{ll}
\text{minimize} & \|Ax - y\|^2 \\
\text{subject to} & \|x\|^2 \le r^2.
\end{array}
$$

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$$\begin{array}{ll} \text{minimize} & \|Ax - y\|^2 \\ \text{subject to} & \|x\|^2 \leq r^2. \end{array}$$

Example

Let $u, v \in \mathbb{R}^n$ such that $\|v\| = 1$. Solve:

$$\begin{array}{ll} \text{minimize} & \|x-u\|^2 \\ \text{subject to} & x \perp v. \end{array}$$

Example

Questions?

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