

Machine Learning Algorithms - Convex analysis

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Motivations

Why do we care about convexity?

- ▶ Local optimal solutions are also global optimal solutions
- ▶ Derive inequality/bounds
(for example remember that we used $\log u \leq u - 1$)

Applications

- ▶ Loss functions
- ▶ Regularization functions
- ▶ Prediction functions (later)

=> study the properties of these functions to derive algorithms

Convex sets and functions

Sets

Convex set

A set $U \subseteq \mathbb{R}^n$ is convex if and only if:

$$\forall \mathbf{u}, \mathbf{u}' \in U, \epsilon \in [0, 1] : \underbrace{\epsilon \mathbf{u} + (1 - \epsilon) \mathbf{u}'}_{\text{convex combination}} \in U$$

Convex hull

The convex hull of a set U , denoted $\mathbf{conv} U$, is the smallest convex set that contains U .

$$\mathbf{conv} U = \{ \epsilon \mathbf{u} + (1 - \epsilon) \mathbf{u}' \mid \mathbf{u}, \mathbf{u}' \in U \text{ and } \epsilon \in [0, 1] \}$$

Example: $\mathbf{conv} E(k) = \Delta(k)$

Functions

Convex function (synthetic definition)

A function $f : U \rightarrow \mathbb{R}$ is convex if and only if:

1. U is a convex set ;
2. $\forall \mathbf{u}, \mathbf{u}' \in U, \epsilon \in [0, 1]$:

$$f\left(\underbrace{\epsilon \mathbf{u} + (1 - \epsilon) \mathbf{u}'}_{\text{dom. needs to be conv.}}\right) \leq \epsilon f(\mathbf{u}) + (1 - \epsilon) f(\mathbf{u}')$$

Concave function

A function f is concave if and only $-f$ is convex.

Functions

Strictly convex function

A function $f : U \rightarrow \mathbb{R}$ is strictly convex if and only if:

1. U is a convex set ;
2. $\forall \mathbf{u}, \mathbf{u}' \in U$ s.t. $\mathbf{u} \neq \mathbf{u}'$, $\epsilon \in]0, 1[$:

$$f\left(\underbrace{\epsilon \mathbf{u} + (1 - \epsilon) \mathbf{u}'}\right) < \epsilon f(\mathbf{u}) + (1 - \epsilon) f(\mathbf{u}')$$

dom. needs to be conv.

Functions

Hessian

Let $f : U \rightarrow \mathbb{R}$ be a twice differentiable function, where $U \subseteq \mathbb{R}^n$.

The Hessian of f at $\mathbf{u} \in U$ is defined as:

$$\nabla^2 f(\mathbf{u}) = \begin{bmatrix} \frac{\partial}{\partial u_1} \frac{\partial}{\partial u_1} f(\mathbf{u}), & \frac{\partial}{\partial u_1} \frac{\partial}{\partial u_2} f(\mathbf{u}), & \dots \\ \frac{\partial}{\partial u_2} \frac{\partial}{\partial u_1} f(\mathbf{u}), & \ddots & \\ \vdots & & \ddots \end{bmatrix},$$

that is: $[\nabla^2 f(\mathbf{u})]_{i,j} = \frac{\partial}{\partial u_i} \frac{\partial}{\partial u_j} f(\mathbf{u})$

Functions

Positive semi-definite matrix

A matrix $\mathbf{H} \in \mathbb{R}^{n \times n}$ is pos. semi-def. if and only if:

$$\forall \mathbf{u} \in \mathbb{R}^n : \quad \langle \mathbf{u}, \mathbf{H}\mathbf{u} \rangle \geq 0$$

Convex function (analytic definition)

A differentiable function $f : U \rightarrow \mathbb{R}$ is convex if and only if:

1. $U \subset \mathbb{R}^n$ is a convex set ;
2. $\forall \mathbf{u} \in U : \nabla^2 f(\mathbf{u})$ is a pos. semi-def. matrix.

If $n = 1$, the second definition simplifies to $\forall \mathbf{u} \in U : f''(\mathbf{u}) \geq 0$

Other important properties

Proper function

A $f : U \rightarrow \mathbb{R} \cup \{-\infty, +\infty\}$ is proper if and only if:

1. $\forall \mathbf{u} \in U : f(\mathbf{u}) \neq -\infty,$
2. $\exists \mathbf{u} \in U$ s.t. $f(\mathbf{u}) \neq +\infty.$

Closed function

A function is closed if and only if its epigraph is closed. This property is equivalent to lower semi-continuity.

\Rightarrow You can simply ignore this for this course.

Extended real value extension

Let $f : U \rightarrow \mathbb{R}$, $U \subseteq \mathbb{R}^n$ be a function.

The e.r.v. extension of f is the function $\tilde{f} : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$ defined as follows:

$$\tilde{f}(\mathbf{u}) = \begin{cases} f(\mathbf{u}) & \text{if } \mathbf{u} \in U, \text{ or equivalently } \mathbf{u} \in \mathbf{dom} f, \\ +\infty & \text{otherwise.} \end{cases}$$

We define $\mathbf{dom} \tilde{f} = \{\mathbf{u} \in \mathbb{R}^n \mid \tilde{f}(\mathbf{u}) \neq \infty\}$.

Property

If f is convex, then \tilde{f} is also convex (to prove).

Notation

In general, we just assume we directly manipulate the e.r.v. extension, i.e. $f = \tilde{f}$.

Extended real value extension

Indicator function

Let S be a set. The indicator function of S is defined as:

$$\delta_S(\mathbf{s}) = \begin{cases} 0 & \text{if } \mathbf{s} \in S, \\ +\infty & \text{otherwise.} \end{cases}$$

Application

Transform a constrained optimization problem into an “unconstrained” problem:

$$\begin{aligned} \min_{\mathbf{u} \in \mathbb{R}^n} f(\mathbf{u}) &= \min_{\mathbf{u} \in \mathbb{R}^n} f(\mathbf{u}) + \delta_S(\mathbf{u}) \\ \text{s.t. } \mathbf{u} &\in S \end{aligned}$$

Operations preserving convexity and closedness

Operations on set of functions

Weighted sum of functions (Beck, th. 2.7 & 2.16)

Let $f_i : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$, $i \in \{1, \dots, m\}$, be a set of convex (closed) functions, and $\alpha_1, \dots, \alpha_m \geq 0$.

Then, the function $f(\mathbf{u}) = \sum_{i=1}^m \alpha_i f_i(\mathbf{u})$ is convex (closed).

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Maximum of functions (Beck, th. 2.7 & 2.16)

Let $f_i : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$, $i \in \{1, \dots, m\}$, be a set of convex (closed) functions. Then, the function $f(\mathbf{u}) = \max(f_1(\mathbf{u}), \dots, f_m(\mathbf{u}))$ is convex (closed).

Example: maximum of affine functions.

Linear transformation (Beck, th. 2.7 & 2.16)

Let:

- ▶ $\mathbf{A} \in \mathbb{R}^{m \times n}$,
- ▶ $\mathbf{b} \in \mathbb{R}^m$,
- ▶ $f : \mathbb{R}^m \rightarrow \mathbb{R} \cup \{\infty\}$ be a convex (closed) function.

Then, the function $h : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$ defined as follows:

$$h(\mathbf{u}) = f(\mathbf{A}\mathbf{u} + \mathbf{b})$$

is convex.

Gradients

Scalar input

Derivative

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a function and $u, w \in \mathbb{R}$ be variables such that:

$$w = f(u).$$

For a given u , how does an infinitesimal change of u impact w ?

Scalar input

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$$\frac{\partial w}{\partial u} = f'(u) = \lim_{\epsilon \rightarrow 0} \frac{f(u + \epsilon) - f(u)}{\epsilon}$$

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Linear approximation

Let $h : \mathbb{R} \rightarrow \mathbb{R}$ be function parameterized by $a \in \mathbb{R}$ defined as follows:

$$h_a(u) = f(a) + f'(a) \cdot (u - a)$$

Then, h_a is an approximation of f for u “close to” a .

Scalar input

Example

$$f(u) = u^2 + 2$$

$$f'(u) = 2u$$

$$h_a(u) = f(a) + f'(a) \cdot (u - a)$$

$$= a^2 + 2 + 2a(u - a)$$

$$= 2au + 2 - a^2$$

Scalar input

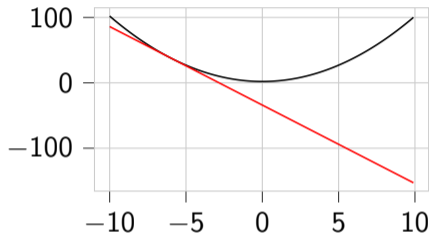
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$$\begin{aligned}h_a(u) &= f(a) + f'(a) \cdot (u - a) \\ &= a^2 + 2 + 2a(u - a) \\ &= 2au + 2 - a^2\end{aligned}$$

Intuition: the sign of $f'(u)$ gives the slope of the approximation, we could use this information to move closer to the minimum of $f(u)$.



- ▶ $a = -6$
- ▶ Black: $f(u)$
- ▶ Red: $h_{-6}(u)$

Scalar input

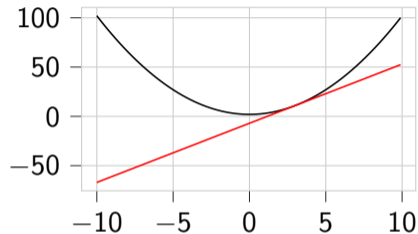
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$$\begin{aligned}h_a(u) &= f(a) + f'(a) \cdot (u - a) \\ &= a^2 + 2 + 2a(u - a) \\ &= 2au + 2 - a^2\end{aligned}$$

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- ▶ $a = 3$
- ▶ Black: $f(u)$
- ▶ Red: $h_3(u)$

Scalar input

Chain rule

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ and $h : \mathbb{R} \rightarrow \mathbb{R}$ be two functions and u, v, w be variables such that:

$$\begin{aligned}v &= f(u), \\w &= h(v) \quad \text{i.e. } w = h(f(u)) = h \circ f(u).\end{aligned}$$

For a given u , how does an infinitesimal change of u impact w ?

Scalar input

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$$\frac{\partial w}{\partial u} = \frac{\partial w}{\partial v} \cdot \frac{\partial v}{\partial u}$$

Scalar input

Example: explicit differentiation

$$f(u) = (2u + 1)^2 = 4u^2 + 4u + 1$$

$$f'(u) = 8u + 4$$

Example: differentiation using the chain rule

$$v = 2u + 1$$

$$\frac{\partial v}{\partial u} = 2$$

$$w = v^2 = f(u)$$

$$\frac{\partial w}{\partial v} = 2v$$

$$\frac{\partial w}{\partial u} = \frac{\partial w}{\partial v} \cdot \frac{\partial v}{\partial u} = 2v * 2 = 4(2u + 1) = 8u + 4 = f'(u)$$

Vector input

Let $f : \mathbb{R}^m \rightarrow \mathbb{R}$ be a function and $\mathbf{u} \in \mathbb{R}^m, w \in \mathbb{R}$ be variables such that:

$$w = f(\mathbf{u}).$$

Partial derivative

For a given \mathbf{u} , how does an infinitesimal change of u_i impact w ?

$$\frac{\partial w}{\partial u_i}$$

i.e. each input $u_j, j \neq i$ is considered as a constant.

Gradient

For a given \mathbf{u} , how does an infinitesimal change of \mathbf{u} impact w ?

$$\nabla_{\mathbf{u}} f(\mathbf{u}) = \begin{bmatrix} \frac{\partial}{\partial u_1} f(\mathbf{u}) \\ \frac{\partial}{\partial u_2} f(\mathbf{u}) \\ \vdots \end{bmatrix}$$

Vector input

Chain rule

Let $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$ and $h : \mathbb{R}^n \rightarrow \mathbb{R}$ be two functions and $\mathbf{u}^m, \mathbf{v}^n, w$ be variables such that:

$$\begin{aligned}\mathbf{v} &= f(\mathbf{u}), \\ w &= h(\mathbf{v})\end{aligned}$$

For a given u_i , how does an infinitesimal change of u_i impact w ?

$$\frac{\partial w}{\partial u_i} = \sum_j \frac{\partial w}{\partial v_j} \cdot \frac{\partial v_j}{\partial u_i}$$

Vector example

$$\mathbf{v} = \mathbf{W}\mathbf{u} + b \quad \text{or} \quad v_j = \sum_i W_{j,i} u_i + b_j$$

$$w = \sum_j v_j$$

$$\frac{\partial v_j}{\partial u_i} = W_{j,i}$$

$$\frac{\partial w}{\partial v_j} = 1$$

$$\frac{\partial w}{\partial u_i} = \sum_j \frac{\partial w}{\partial v_j} \cdot \frac{\partial v_j}{\partial u_i} = \sum_j 1 * W_{j,i}$$

Subgradients

Subgradient

Given a function $f : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$, a subgradient at $\mathbf{u} \in U$ is a vector $\mathbf{g} \in \mathbb{R}^n$ such that:

$$\forall \mathbf{u}' \in \mathbb{R}^n : f(\mathbf{u}') \geq f(\mathbf{u}) + \langle \mathbf{g}, \mathbf{u}' - \mathbf{u} \rangle$$

The set of subgradients at point \mathbf{u} is called the subdifferential and is denoted $\partial f(\mathbf{u})$.

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Properties

If f is convex, then:

- ▶ if f is differentiable at \mathbf{u} , then $\partial f(\mathbf{u}) = \{\nabla f(\mathbf{x})\}$
(i.e. the gradient is the single subgradient)
- ▶ the function $h(\mathbf{u}') = f(\mathbf{u}) + \langle \mathbf{g}, \mathbf{u}' - \mathbf{u} \rangle$ is a linear sub-estimator of f
- ▶ a similar definition for concave function is the super-gradient

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- ▶ a similar definition for concave function is the super-gradient

Existence of the subgradient (Beck, th. 3.14)

Let f be a proper convex function.

Then, $\forall \mathbf{u} \in \text{int}(\text{dom } f)$, the subdifferential $\partial f(\mathbf{u})$ is non-empty.

Computing subgradients 1/2

There are "rules" that allows to compute the subgradient of a function at a given point (see Beck, Section 2.4).

- ▶ Strong subgradient result: the subdifferential set at a given point is known
- ▶ Weak subgradient result: one or several subgradients at a given point are known, but not all

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Multiplication by a positive scalar (Beck, th. 3.35)

Let $f : \mathbb{R}^k \rightarrow \mathbb{R} \cup \{\infty\}$ be a proper function, $h(\mathbf{u}) = \alpha f(\mathbf{u})$ with $\alpha > 0$. Then:

$$\forall \mathbf{u} \in \text{dom } f, \mathbf{g} \in \mathbb{R}^k : \alpha \mathbf{u} \in \partial h(\mathbf{u}) \quad \text{if and only if} \quad \mathbf{g} \in \partial f(\mathbf{u})$$

Computing subgradients 2/2

Summation (Beck, th. 3.36)

Let $f_1 : \mathbb{R}^k \rightarrow \mathbb{R} \cup \{\infty\}$ and $f_2 : \mathbb{R}^k \rightarrow \mathbb{R} \cup \{\infty\}$ be proper functions and $h(\mathbf{u}) = f_1(\mathbf{u}) + f_2(\mathbf{u})$. Then, $\forall \mathbf{u} \in \text{dom } h, \mathbf{g} \in \mathbb{R}^k$, we have $\mathbf{g} \in \partial h(\mathbf{u})$ if and only if:

$$\mathbf{g} = \mathbf{g}^{(1)} + \mathbf{g}^{(2)} \quad \text{such that} \quad \mathbf{g}^{(1)} \in \partial f_1(\mathbf{u}) \text{ and } \mathbf{g}^{(2)} \in \partial f_2(\mathbf{u})$$

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Let $f_1 : \mathbb{R}^k \rightarrow \mathbb{R} \cup \{\infty\}$ and $f_2 : \mathbb{R}^k \rightarrow \mathbb{R} \cup \{\infty\}$ be proper functions and $h(\mathbf{u}) = f_1(\mathbf{u}) + f_2(\mathbf{u})$. Then, $\forall \mathbf{u} \in \text{dom } h$, $\mathbf{g} \in \mathbb{R}^k$, we have $\mathbf{g} \in \partial h(\mathbf{u})$ if and only if:

$$\mathbf{g} = \mathbf{g}^{(1)} + \mathbf{g}^{(2)} \quad \text{such that} \quad \mathbf{g}^{(1)} \in \partial f_1(\mathbf{u}) \text{ and } \mathbf{g}^{(2)} \in \partial f_2(\mathbf{u})$$

Maximization (Beck, th. 3.50)

Let $f_1 \dots f_n : \mathbb{R}^k \rightarrow \mathbb{R} \cup \{\infty\}$ be a set of proper functions and

$$h(\mathbf{u}) = \max(f_1(\mathbf{u}), \dots, f_n(\mathbf{u}))$$

Let $\mathbf{u} \in \mathbb{R}^k$ and $I(\mathbf{u}) = \{i \in \{1 \dots n\} \mid f_i(\mathbf{u}) = h(\mathbf{u})\}$.

If $\mathbf{g} \in \partial f_i(\mathbf{u})$ for any $i \in I(\mathbf{u})$, then $\mathbf{g} \in \partial h(\mathbf{u})$.

(Note: we could get stronger result than this)

Optimality conditions

Unconstrained optimization problem (Fermat's theorem)

Let $f : \mathbb{R}^k \rightarrow \mathbb{R} \cup \{\infty\}$ be a proper convex function and $\hat{\mathbf{u}} \in \mathbf{dom} f$.
If $0 \in \partial f(\hat{\mathbf{u}})$,
then $f(\hat{\mathbf{u}})$ is the global minimum of f .

Proof

By the subgradient definition:

$$\forall \mathbf{u} \in \mathbb{R}^k, \mathbf{g} \in \partial f(\hat{\mathbf{u}}) : f(\mathbf{u}) \geq f(\hat{\mathbf{u}}) + \langle \mathbf{g}, \mathbf{u} - \hat{\mathbf{u}} \rangle$$

In particular, we know that $0 \in \partial f(\hat{\mathbf{u}})$, therefore:

$$f(\mathbf{u}) \geq f(\hat{\mathbf{u}})$$

Fenchel conjugates

Definition

Let $f : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$ be a function.

The Fenchel conjugate of f is the function $f^* : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$ defined as follows:

$$f^*(\mathbf{t}) = \sup_{\mathbf{u} \in \text{dom } f} \langle \mathbf{t}, \mathbf{u} \rangle - f(\mathbf{u})$$

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The biconjugate of f is the function $f^{**} : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{\infty\}$ defined as follows:

$$f^{**}(\mathbf{u}) = \sup_{\mathbf{t} \in \text{dom } f^*} \langle \mathbf{u}, \mathbf{t} \rangle - f^*(\mathbf{t})$$

If f is proper, closed and convex, then $f^{**} = f$

\Rightarrow important property is often used to build variational formulation of functions

One small theorem

Fenchel-Young inequality

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a function, $\mathbf{u} \in \mathbf{dom} f$ and $\mathbf{t} \in \mathbf{dom} f^*$:

$$f(\mathbf{u}) + f^*(\mathbf{t}) \geq \langle \mathbf{u}, \mathbf{t} \rangle$$

Proof

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a function, $\mathbf{u} \in \mathbf{dom} f$ and $\mathbf{t} \in \mathbf{dom} f^*$:

$$\begin{aligned} \langle \mathbf{u}, \mathbf{t} \rangle - f(\mathbf{u}) &\leq \sup_{\mathbf{u}' \in \mathbf{dom} f} \mathbf{u}'^\top \mathbf{t} - f(\mathbf{u}') \\ &= f^*(\mathbf{t}) \end{aligned}$$

By re-arranging terms we get the expected inequality.

Subdifferential of a Fenchel conjugate

Let $f : \mathbb{R}^k \rightarrow \mathbb{R} \cup \{\infty\}$ be function. Let $\mathbf{t} \in \mathbf{dom} f^*$ and

$$\hat{\mathbf{u}} = \arg \max_{\mathbf{u} \in \mathbf{dom} f} \langle \mathbf{u}, \mathbf{t} \rangle - f(\mathbf{u})$$

Then, $\hat{\mathbf{u}}$ is a subgradient of f^* at \mathbf{t} , i.e. $\hat{\mathbf{u}} \in \partial f^*(\mathbf{t})$.

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Then, $\hat{\mathbf{u}}$ is a subgradient of f^* at \mathbf{t} , i.e. $\hat{\mathbf{u}} \in \partial f^*(\mathbf{t})$.

Proof

Although this can be proved via Danskin's theorem, here is a simpler proof.

We have $f^*(\mathbf{t}) = \max_{\mathbf{u} \in \mathbf{dom} f} \langle \mathbf{u}, \mathbf{t} \rangle - f(\mathbf{u}) = \langle \hat{\mathbf{u}}, \mathbf{t} \rangle - f(\hat{\mathbf{u}})$.

For all $\mathbf{t}' \in \mathbf{dom} f^*$ we have:

$$\begin{aligned} f^*(\mathbf{t}) + \langle \hat{\mathbf{u}}, \mathbf{t}' - \mathbf{t} \rangle &= \langle \hat{\mathbf{u}}, \mathbf{t} \rangle - f(\hat{\mathbf{u}}) + \langle \hat{\mathbf{u}}, \mathbf{t}' \rangle - \langle \hat{\mathbf{u}}, \mathbf{t} \rangle \\ &= \langle \hat{\mathbf{u}}, \mathbf{t}' \rangle - f(\hat{\mathbf{u}}) \\ &\leq \max_{\mathbf{u} \in \mathbf{dom} f} \mathbf{u}^\top \mathbf{t}' - f(\mathbf{u}) \\ &= f^*(\mathbf{t}') \end{aligned}$$

Hence $\hat{\mathbf{u}}$ is a subgradient of f^* at \mathbf{t} .